Scientific and Technical Information Center

Requester's Full Name: Berch 09/929771 Examiner #: 59193 Date: 3/20/03
Art Unit: 1624 Phone Number 30 84718 Serial Number: 09/929271
Mail Box and Bldg/Room Location: 4E12 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need. ME

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

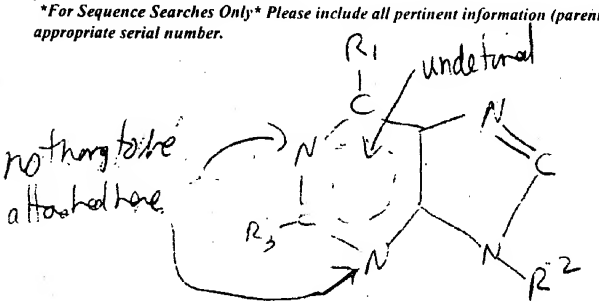
Inventors (please provide full names): _____

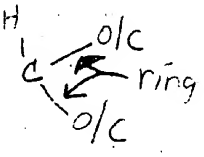
_____

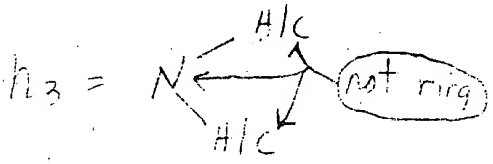
Earliest Priority Filing Date: _____

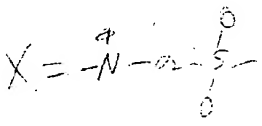
For Sequence Searches Only *Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

NO PY 2000-2003 (1999 or earlier)



R^2 = C, but not 

R_3 = 

X = 

R4 — same definition as R_2

$R_1 = -X-R_4$

****

STAFF USE ONLY

Point of Contact:
Alexandra Waclawiw
Technical Info. Specialist
CM1 8A02 Tel: 308-4491

Searcher: _____
Searcher Phone #: _____
Searcher Location: _____
Date Searcher Picked Up: 3.24.03
Date Completed: 3.24.03
Searcher Prep & Review Time: 15
Clerical Prep Time: _____
Online Time: 37

Type of Search		Vendors and cost where applicable	
NA Sequence (#)		STN	5 + 3.30
AA Sequence (#)		Dialog	
Structure (#)	1	Questel/Orbit	
Bibliographic		Dr.Link	
Litigation		Lexis/Nexis	
Fulltext		Sequence Systems	
Patent Family		WWW/Internet	
Other		Other (specify)	

PTO-1590 (8-01)

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=> d his

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               ACT BERCH2/A
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L1             STR
L2           953 SEA FILE=REGISTRY SSS FUL L1
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     FILE 'HCAPLUS' ENTERED AT 09:11:34 ON 24 MAR 2003
L3           248 S L2
L4            92 S L3 NOT (2000-2003)/PY
L5            40 S L2/P AND L4
               SELEC HIT RN L5 1-40

=> fil reg
FILE 'REGISTRY' ENTERED AT 09:12:41 ON 24 MAR 2003
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STRUCTURE FILE UPDATES:   23 MAR 2003  HIGHEST RN 500280-37-5
DICTIONARY FILE UPDATES:  23 MAR 2003  HIGHEST RN 500280-37-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

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L1               STR
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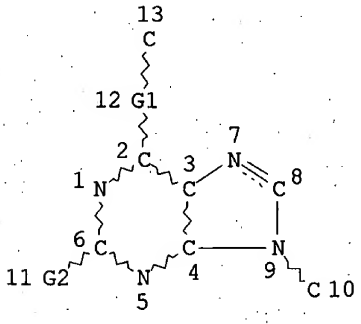

NH~C
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C~N~C
16 @17 18

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CONNECT IS E2  RC AT   5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  18

STEREO ATTRIBUTES: NONE
L2          953 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED   8038 ITERATIONS                    953 ANSWERS
SEARCH TIME: 00.00.01


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FILE 'HCAPLUS' ENTERED AT 09:12:51 ON 24 MAR 2003
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FILE COVERS 1907 - 24 Mar 2003  VOL 138 ISS 13
FILE LAST UPDATED: 23 Mar 2003  (20030323/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

=> d his l3-

     (FILE 'REGISTRY' ENTERED AT 09:11:25 ON 24 MAR 2003)
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     FILE 'HCAPLUS' ENTERED AT 09:11:34 ON 24 MAR 2003
L3          248 S L2
L4           92 S L3 NOT (2000-2003)/PY
L5           40 S L2/P AND L4
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SELEC HIT RN L5 1-40

FILE 'REGISTRY' ENTERED AT 09:12:41 ON 24 MAR 2003

FILE 'HCAPLUS' ENTERED AT 09:12:51 ON 24 MAR 2003

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L3           248 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L2
L4            92 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3 NOT (2000-2003)/PY
L5            40 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L2/P AND L4

=> d .ca hitstr l5 1-40

L5   ANSWER 1 OF 40  HCAPLUS  COPYRIGHT 2003 ACS
ACCESSION NUMBER:        1999:485959  HCAPLUS
DOCUMENT NUMBER:         131:310491
TITLE:                   Synthesis and in vitro evaluation of novel
                         2,6,9-trisubstituted purines acting as
                         cyclin-dependent kinase inhibitors
AUTHOR(S):               Legraverend, Michel; Ludwig, Odile; Bisagni, Emile;
                         Leclerc, Sophie; Meijer, Laurent; Giocanti, Nicole;
                         Sadri, Ramin; Favaudon, Vincent
CORPORATE SOURCE:        UMR 176 CNRS-IC, Institut Curie-Recherche, Centre
                         Universitaire, Orsay, 91405, Fr.
SOURCE:                  Bioorganic & Medicinal Chemistry (1999), 7(7),
                         1281-1293
                         CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER:               Elsevier Science Ltd.
DOCUMENT TYPE:           Journal
LANGUAGE:                English
GI
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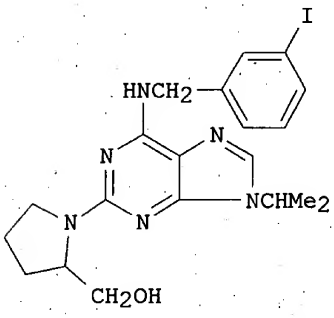


I

AB Novel C-2, C-6, N-9 trisubstituted purines derived from the olomoucine/roscovitine lead structure were synthesized and evaluated for their ability to inhibit starfish oocyte CDK1/cyclin B, neuronal CDK5/p35 and erk1 kinases in purified exts. Structure-activity relationship studies showed that increased steric bulk at N-9 reduces the inhibitory potential whereas substitution of the aminoethanol C-2 side chain by various groups of different size (Me, Pr, Bu, Ph, benzyl) only slightly

decreases the activity when compared to (R)-roscovitine. Optimal inhibitory activity against CDK5, CDK1 and CDK2, with IC50 values of 0.16, 0.45 and 0.65 .mu.M, resp., was obtained with compd. I contg. a (2R)-pyrrolidin-2-yl-methanol substituent at the C-2 and a 3-iodobenzylamino group at the C-6 of the purine. I proved cytotoxic against human tumor HeLa cells (LD50=6.7 .mu.M vs. 42.7 .mu.M for olomoucine, 24-h contact). Furthermore, unlike olomoucine, I was effective upon short exposure (LD50=25.3 .mu.M, 2-h contact). The available data suggest that the affinity for CDKs and the cytotoxic potential of the drugs are inter-related. However, no straightforward cell cycle phase specificity of the cytotoxic response to I was obsd. in synchronized HeLa cells. With the noticeable exception of pronounced lengthening of the S-phase transit by I applied during early-S in synchronized HeLa cells, and in striking contrast with earlier reports on studies using plant or echinoderm cells, olomoucine and I were unable to reversibly arrest cell cycle progression in asynchronous growing HeLa cells. Some irreversible block in G1 and G2 phase occurred at high olomoucine concn., correlated with induced cell death. Moreover, chronic exposure to LDs of I resulted in massive nuclear fragmentation, evocative of mitotic catastrophe with minor amts. of apoptosis only. It was also found that olomoucine and I reversibly block the intracellular uptake of nucleosides with high efficiency.

CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 7

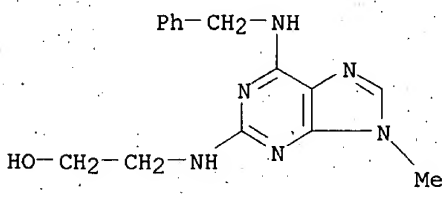
IT **101622-51-9 186692-44-4 186692-46-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(prepn. and in vitro activity of 2,6,9-trisubstituted purines as cyclin-dependent kinase inhibitors)

IT 192327-96-1P **192327-97-2P 192327-98-3P**
192327-99-4P 192328-00-0P 192328-01-1P
192328-02-2P 192328-03-3P 192328-04-4P
192328-05-5P 192328-06-6P **247193-47-1P 247193-48-2P**
247193-49-3P 247193-50-6P **247193-52-8P 247193-53-9P**
247193-55-1P 247193-56-2P 247193-58-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and in vitro activity of 2,6,9-trisubstituted purines as cyclin-dependent kinase inhibitors)

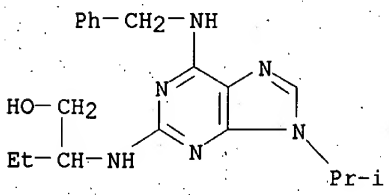
IT **101622-51-9 186692-44-4 186692-46-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(prepn. and in vitro activity of 2,6,9-trisubstituted purines as cyclin-dependent kinase inhibitors)

RN 101622-51-9 HCAPLUS

CN Ethanol, 2-[[9-methyl-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)

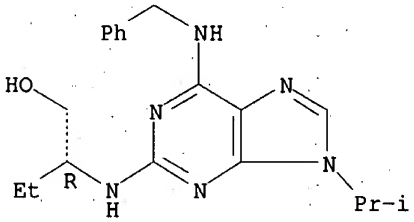


RN 186692-44-4 HCAPLUS
CN 1-Butanol, 2-[[9-(1-methylethyl)-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



RN 186692-46-6 HCAPLUS
CN 1-Butanol, 2-[[9-(1-methylethyl)-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



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192328-03-3P 192328-04-4P 247193-47-1P
247193-48-2P 247193-52-8P 247193-53-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and in vitro activity of 2,6,9-trisubstituted purines as cyclin-dependent kinase inhibitors)

RN 192327-97-2 HCAPLUS
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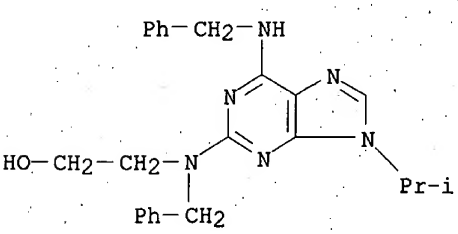

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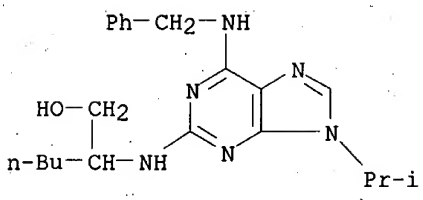

RN 192327-99-4 HCAPLUS
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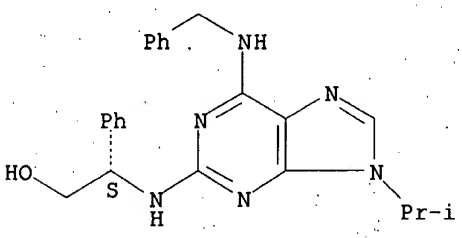
Absolute stereochemistry.



RN 192328-00-0 HCAPLUS
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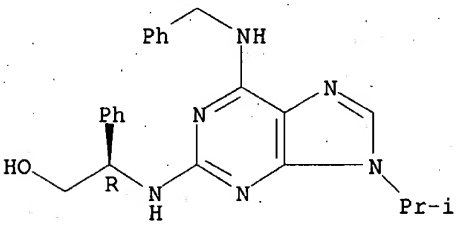
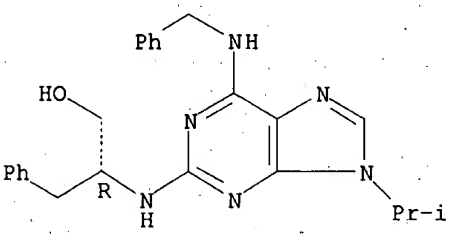
Absolute stereochemistry.

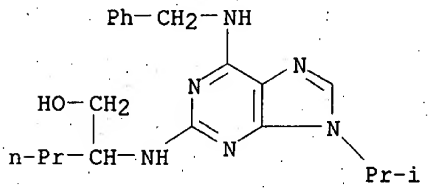


RN 192328-01-1 HCAPLUS
CN Benzenepropanol, .beta.-[[9-(1-methylethyl)-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]-, (.beta.R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 192328-02-2 HCAPLUS
CN 1-Pentanol, 2-[[9-(1-methylethyl)-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



RN 192328-03-3 HCAPLUS
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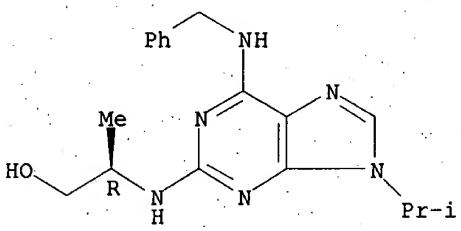
Absolute stereochemistry.



RN 192328-04-4 HCAPLUS
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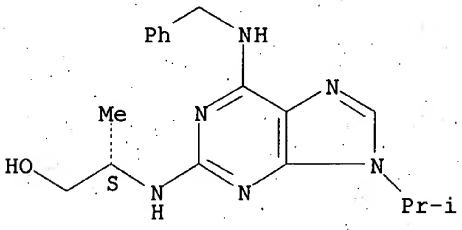
Absolute stereochemistry.



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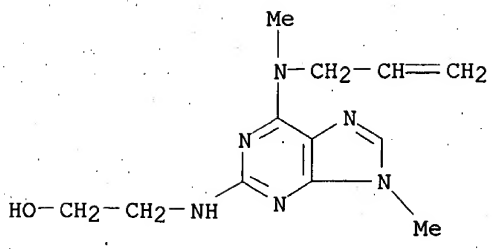

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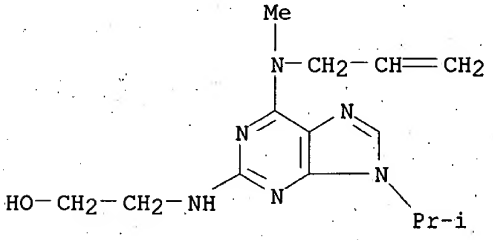

RN 247193-52-8 HCAPLUS
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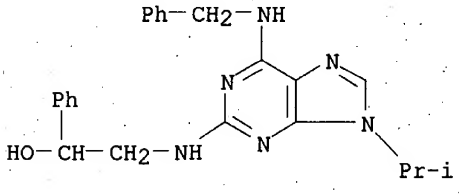
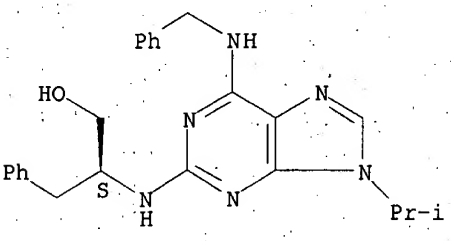


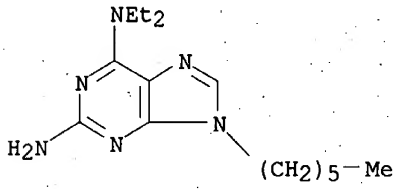
RN 247193-53-9 HCAPLUS
CN Benzenepropanol, .beta.-[[9-(1-methylethyl)-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]-, (.beta.S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:484857 HCAPLUS
DOCUMENT NUMBER: 131:286322
TITLE: Catalysis of Nucleobase via Multiple Hydrogen-Bonding Interactions: Acceleration of Aminolysis of 6-Chloropurine Derivatives by Uracils
AUTHOR(S): Tominaga, Masahide; Konishi, Katsuaki; Aida, Takuzo
CORPORATE SOURCE: Department of Chemistry and Biotechnology Graduate School of Engineering, The University of Tokyo, Bunkyo-ku Tokyo, 113-8656, Japan
SOURCE: Journal of the American Chemical Society (1999), 121(33), 7704-7705
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The aminolysis of 2-amino-6-chloro-9-hexylpurine is catalyzed by uracils with hydrogen-bonding capability.
CC 26-9 (Biomolecules and Their Synthetic Analogs)
IT **246244-68-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(acceleration of aminolysis of 6-chloropurine derivs. by uracils)
IT **246244-68-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(acceleration of aminolysis of 6-chloropurine derivs. by uracils)
RN 246244-68-8 HCAPLUS
CN 9H-Purine-2,6-diamine, N6,N6-diethyl-9-hexyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:397364 HCAPLUS
DOCUMENT NUMBER: 131:228582
TITLE: Synthesis and application of functionally diverse 2,6,9-trisubstituted purine libraries as CDK inhibitors
AUTHOR(S): Chang, Young-Tae; Gray, Nathanael S.; Rosania, Gustavo R.; Sutherlin, Daniel P.; Kwon, Soojin; Norman, Thea C.; Sarohia, Radhika; Leost, Maryse; Meijer, Laurent; Schultz, Peter G.
CORPORATE SOURCE: Lawrence Berkeley National Laboratory and the Howard Hughes Medical Institute, Department of Chemistry, University of California, Berkeley, CA, 94720, USA
SOURCE: Chemistry & Biology (1999), 6(6), 361-375

CODEN: CBOLE2; ISSN: 1074-5521
PUBLISHER: Current Biology Publications
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Purines constitute a structural class of protein ligands involved in mediating an astonishing array of metabolic processes and signal pathways in all living organisms. Synthesis of purine derivs. targeting specific purine-binding proteins in vivo could lead to versatile lead compds. for use as biol. probes or drug candidates. We synthesized several libraries of 2,6,9-trisubstituted purines using both soln.- and solid-phase chem., and screened the compds. for inhibition of cyclin-dependent kinase (CDK) activity and human leukemic cell growth. Lead compds. were optimized by iterative synthesis based on structure-activity relationships (SARs), as well as anal. of several CDK-inhibitor cocrystal structures, to afford several interesting compds. including one of the most potent CDK inhibitors known to date. Unexpectedly, some compds. with similar CDK inhibitory activity arrested cellular proliferation at distinctly different phases of the cell cycle, and another inhibitor directly induced apoptosis, bypassing cell-cycle arrest. Some of these compds. selectively inhibited growth of cells derived from specific tumors. 2,6,9-Trisubstituted purines have various and potent biol. activities, despite high concns. of competing endogenous purine ligands in living cells. Purine libraries constitute a versatile source of small mols. that affect distinct biochem. pathways mediating different cellular functions.

CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 7

IT 190654-60-5P **199986-74-8P 199986-75-9P**
199986-90-8P 199986-95-3P **199987-14-9P**
199987-36-5P 203436-23-1P 203436-24-2P
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220791-11-7P 220791-16-2P **220791-21-9P** 220791-22-0P
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244030-43-1P 244030-44-2P 244030-45-3P 244030-46-4P 244030-47-5P
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244030-70-4P 244030-71-5P 244030-72-6P 244030-73-7P 244030-74-8P
244030-75-9P 244030-76-0P 244030-77-1P 244030-78-2P 244030-79-3P
244030-80-6P 244030-81-7P 244030-82-8P 244030-83-9P 244030-85-1P
244030-86-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and application of functionally diverse 2,6,9-trisubstituted purine libraries as CDK inhibitors)

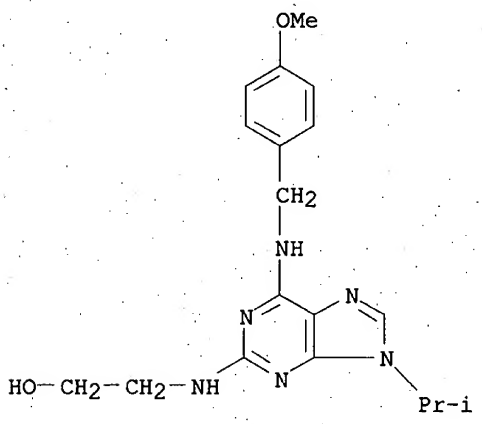
IT 220696-58-2P, 2-Fluoro-6-chloro-9-isopropylpurine 229966-54-5P,
2-Fluoro-6-(3-chloroanilino)-9-isopropylpurine 244030-27-1P,
2-Fluoro-6-chloro-9-[(2-(trimethylsilyl)ethoxy)methyl]purine
244030-28-2P, 2-Amino-6-chloro-9-isopropylpurine 244030-29-3P
244030-30-6P 244030-31-7P **244030-32-8P 244030-33-9P**
244030-84-0P, 2-(Trifluoroacetamido)-6-chloro-9-isopropylpurine

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and application of functionally diverse 2,6,9-trisubstituted purine libraries as CDK inhibitors)

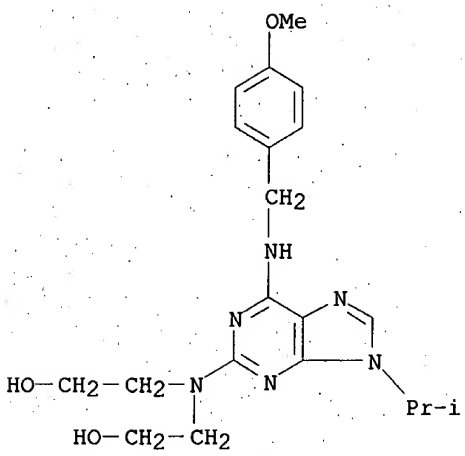
IT **244030-87-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and application of functionally diverse 2,6,9-trisubstituted purine libraries as CDK inhibitors)

IT **199986-74-8P 199986-75-9P 199986-90-8P**
199987-14-9P 199987-36-5P 203436-23-1P
203436-24-2P 203436-32-2P 220791-21-9P
220791-29-7P 220791-34-4P 220791-38-8P
220791-42-4P 220791-52-6P 244030-37-3P
244030-53-3P 244030-55-5P 244030-56-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis and application of functionally diverse 2,6,9-trisubstituted purine libraries as CDK inhibitors)

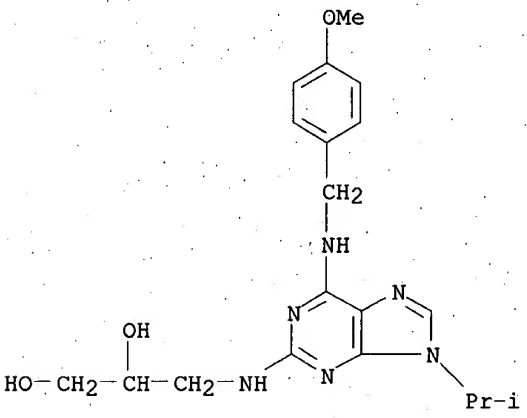
RN 199986-74-8 HCAPLUS
CN Ethanol, 2-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



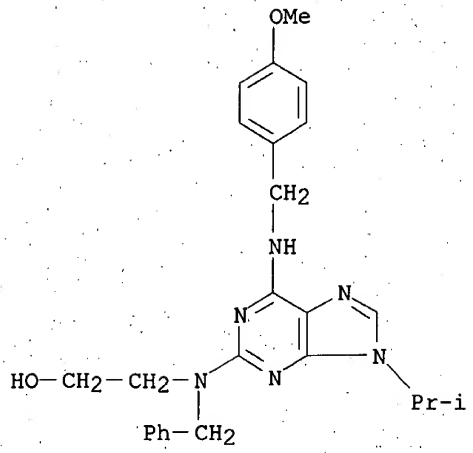
RN 199986-75-9 HCAPLUS
CN Ethanol, 2,2'-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



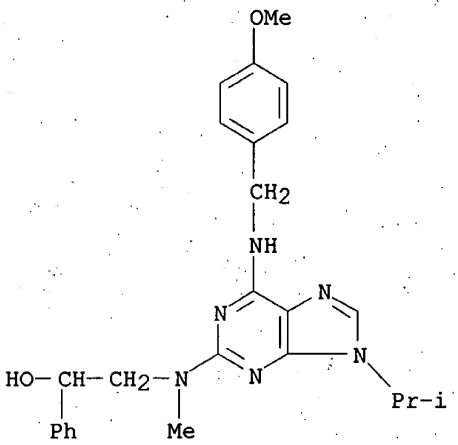
RN 199986-90-8 HCAPLUS
CN 1,2-Propanediol, 3-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



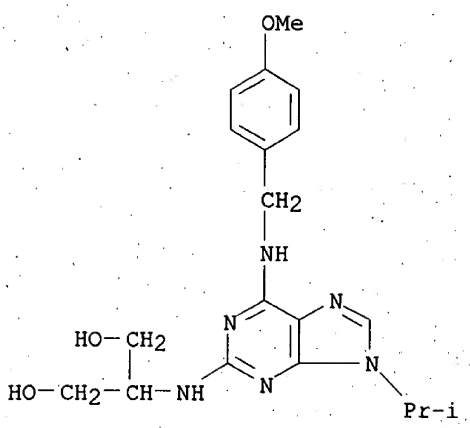
RN 199987-14-9 HCAPLUS
CN Ethanol, 2-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl](phenylmethyl)amino]- (9CI) (CA INDEX NAME)



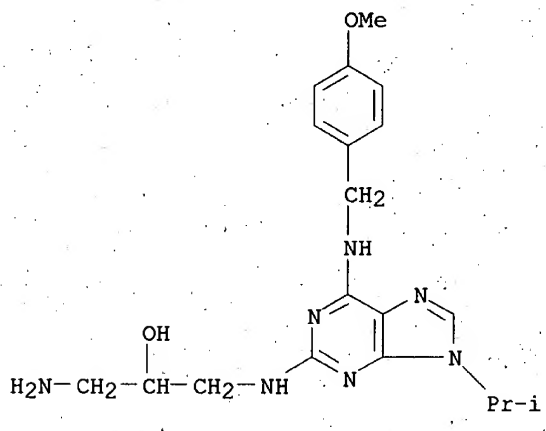
RN 199987-36-5 HCAPLUS
CN Benzenemethanol, .alpha.-[[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]methylamino]methyl]- (9CI) (CA INDEX NAME)



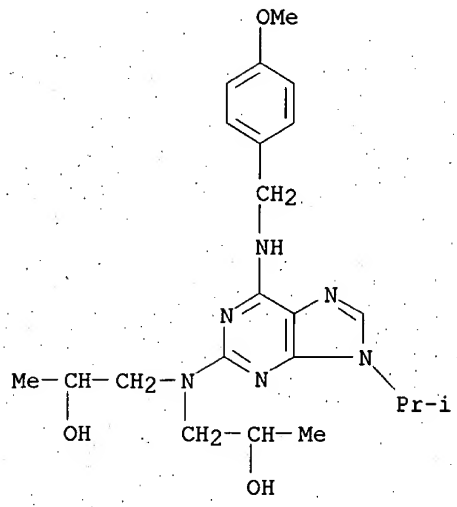
RN 203436-23-1 HCAPLUS
CN 1,3-Propanediol, 2-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



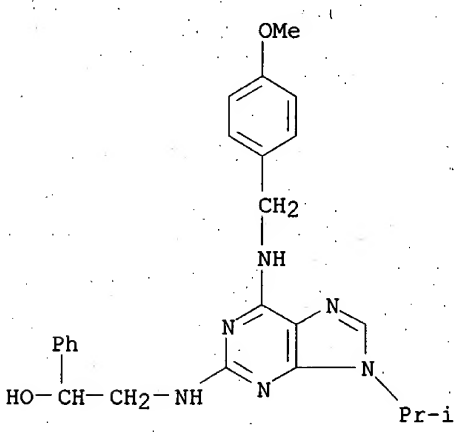
RN 203436-24-2 HCAPLUS
CN 2-Propanol, 1-amino-3-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



RN 203436-32-2 HCAPLUS
CN 2-Propanol, 1,1'-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)

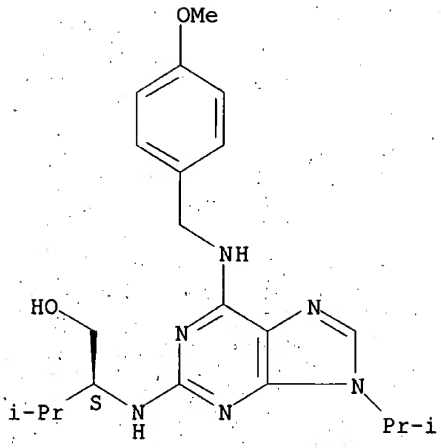


RN 220791-21-9 HCAPLUS
CN Benzenemethanol, .alpha.-[[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]methyl]- (9CI) (CA INDEX NAME)



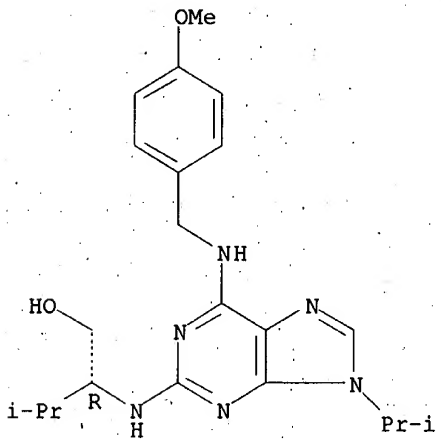
RN 220791-29-7 HCAPLUS
CN 1-Butanol, 2-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-3-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



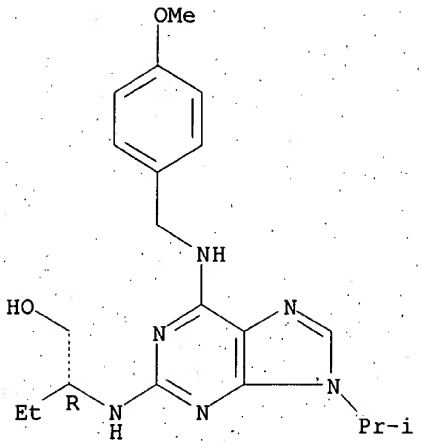
RN 220791-34-4 HCAPLUS
CN 1-Butanol, 2-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-3-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



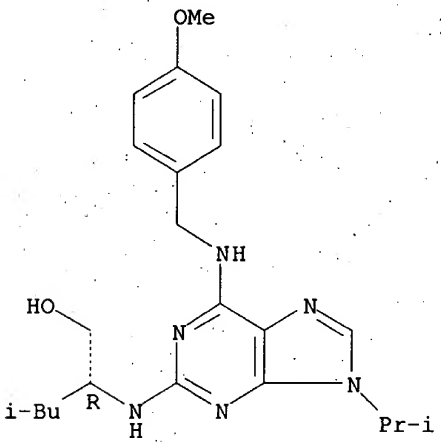
RN 220791-38-8 HCAPLUS
CN 1-Butanol, 2-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

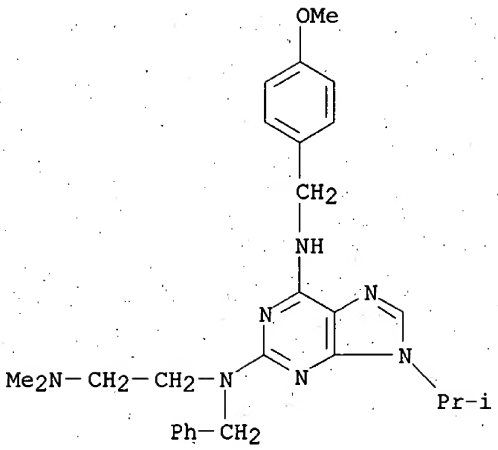


RN 220791-42-4 HCAPLUS
CN 1-Pentanol, 2-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-4-methyl-, (2R)- (9CI) (CA INDEX NAME)

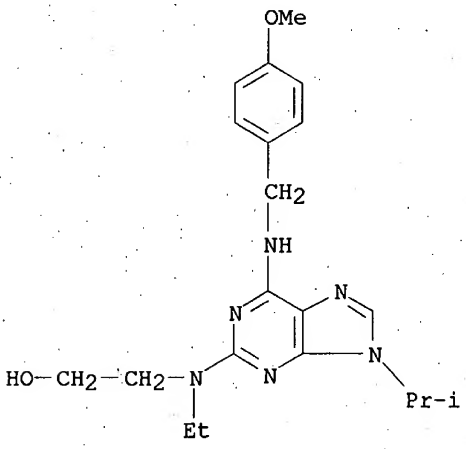
Absolute stereochemistry.



RN 220791-52-6 HCAPLUS
CN 9H-Purine-2,6-diamine, N2-[2-(dimethylamino)ethyl]-N6-[(4-methoxyphenyl)methyl]-9-(1-methylethyl)-N2-(phenylmethyl)- (9CI) (CA INDEX NAME)

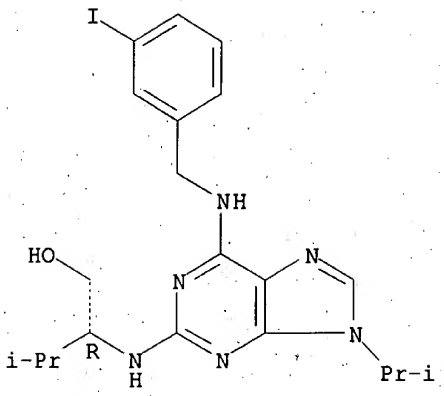


RN 244030-37-3 HCAPLUS
CN Ethanol, 2-[ethyl[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)

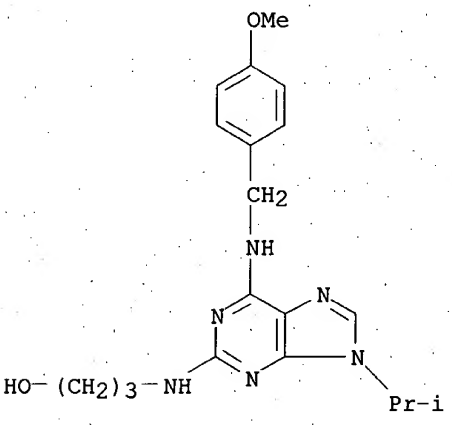


RN 244030-53-3 HCAPLUS
CN 1-Butanol, 2-[[6-[[(3-iodophenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-3-methyl-, (2R)- (9CI) (CA INDEX NAME)

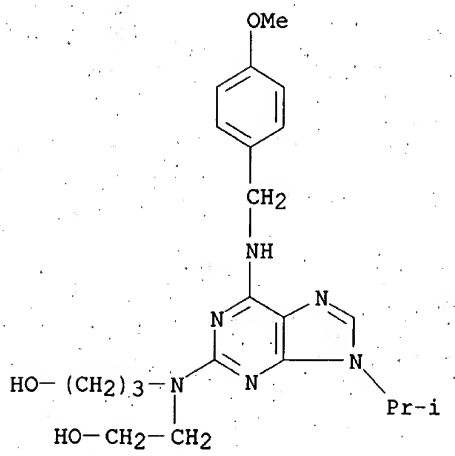
Absolute stereochemistry.



RN 244030-55-5 HCAPLUS
CN 1-Propanol, 3-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



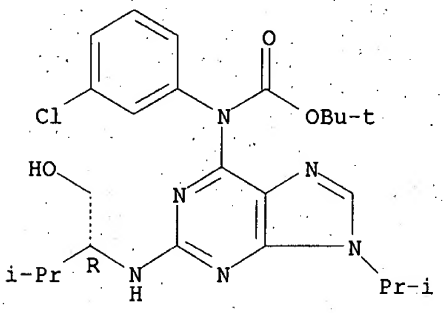
RN 244030-56-6 HCAPLUS
CN 1-Propanol, 3-[(2-hydroxyethyl)[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



IT **244030-32-8P 244030-33-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and application of functionally diverse 2,6,9-trisubstituted purine libraries as CDK inhibitors)

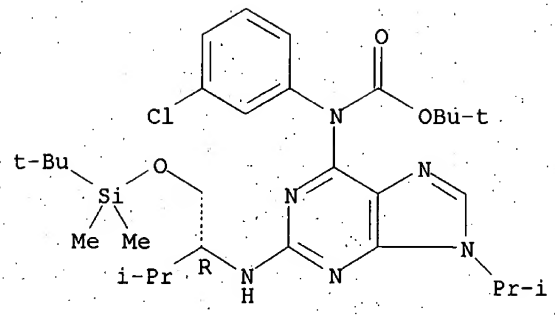
RN 244030-32-8 HCAPLUS
CN Carbamic acid, (3-chlorophenyl)[2-[[(1R)-1-(hydroxymethyl)-2-methylpropyl]amino]-9-(1-methylethyl)-9H-purin-6-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



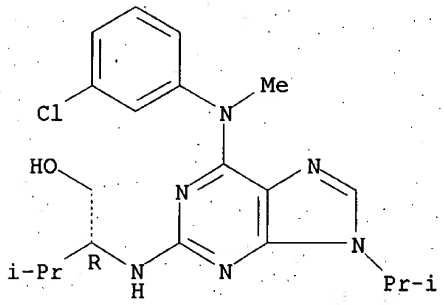
RN 244030-33-9 HCAPLUS
CN Carbamic acid, (3-chlorophenyl)[2-[[(1R)-1-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-2-methylpropyl]amino]-9-(1-methylethyl)-9H-purin-6-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **244030-87-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and application of functionally diverse 2,6,9-trisubstituted purine libraries as CDK inhibitors)
RN 244030-87-3 HCAPLUS
CN 1-Butanol, 2-[[6-[(3-chlorophenyl)methylamino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-3-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:306503 HCAPLUS
DOCUMENT NUMBER: 131:97125
TITLE: A cyclin-dependent kinase inhibitor inducing cancer cell differentiation: biochemical identification using Xenopus egg extracts
AUTHOR(S): Rosania, Gustavo R.; Merlie, John, Jr.; Gray, Nathanael; Chang, Young-Tae; Schultz, Peter G.; Heald, Rebecca
CORPORATE SOURCE: Department of Chemistry and Howard Hughes Medical Institute, University of California, Berkeley, CA, 94720, USA
SOURCE: Proceedings of the National Academy of Sciences of the United States of America (1999), 96(9), 4797-4802
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Cellular differentiation is a complex process involving growth arrest, exit from the cell cycle, and expression of differentiated cell-type-specific functions. To identify small mols. promoting this process, a chem. library was screened by using a myeloid leukemic cell line that retained the potential to differentiate in culture. In the presence of a purine deriv., aminopurvalanol (AP), cells acquired phenotypic characteristics of differentiated macrophages and became arrested in the cell cycle with a 4N DNA content. AP also inhibited mitosis in Xenopus egg exts., suggesting that it acted on an evolutionarily conserved cell cycle regulatory pathway. Affinity chromatog. and biochem. reconstitution expts. with Xenopus egg exts. identified cyclin-dependent kinase (CDK) 1-cyclin B as a target of the compd. Although AP potently inhibited immunoppts. of both human CDK1 and CDK2 from human leukemic cell exts., our results indicate that the compd. preferentially targets the G2/M-phase transition in vivo.

CC 1-6 (Pharmacology)

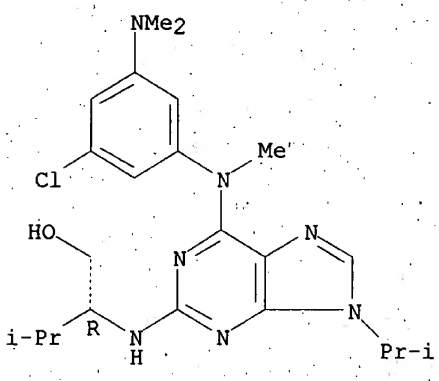
IT **231951-20-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of cyclin-dependent kinase inhibitor inducing cancer cell differentiation)

IT **231951-20-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of cyclin-dependent kinase inhibitor inducing cancer cell differentiation)

RN 231951-20-5 HCAPLUS

CN 1-Butanol, 2-[[6-[[3-chloro-5-(dimethylamino)phenyl]methylamino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-3-methyl-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:589540 HCAPLUS
DOCUMENT NUMBER: 129:276358
TITLE: Preparation of nucleic acid-binding peptides using specific protection/deprotection strategy
INVENTOR(S): Baetz, Hans Georg; Hansen, Henrik Frydenlund; Oerum, Henrik; Koch, Troels; Kofeod, Thomas
PATENT ASSIGNEE(S): Boehringer Mannheim G.m.b.H., Germany
SOURCE: Jpn. Kokai Tokkyo Koho, 25 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

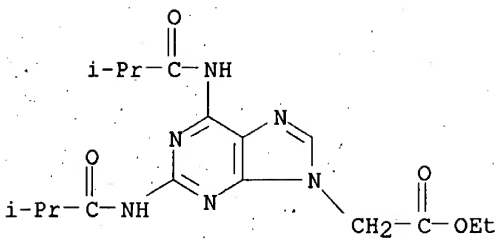
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10231290	A2	19980902	JP 1998-25937	19980206
CA 2228875	AA	19980808	CA 1998-2228875	19980206
EP 863150	A1	19980909	EP 1998-102059	19980206

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

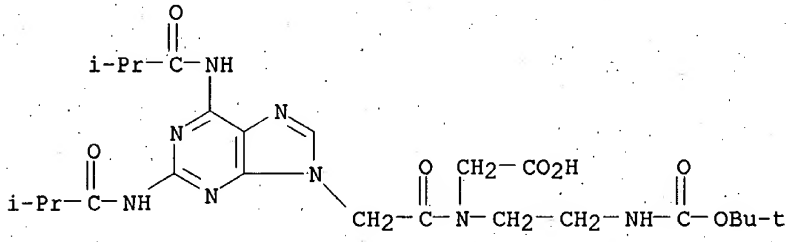
PRIORITY APPLN. INFO.: EP 1997-102028 19970208
OTHER SOURCE(S): MARPAT 129:276358

AB Title peptides are prepd. by (1) prepg. protected compds. having (a) plural ligands, which are bound to backbone, can be linked to bases of nucleic acids via H bond, and have primary or secondary amino group protected by strong-base-removable group and (b) backbones having NX1X2 (X1 = H, C1-3 alkyl, strong-acid-removable protecting group; X2 = strong-acid-removable protecting group), (2) removing the strong-acid-removable groups, and (3) removing the strong-base-removable groups. Two kinds of markers may be bound to the 2 kinds of deprotected amino groups. Monomers for the peptides are also claimed. The peptides are rapidly prepd. in high yield and large scale. The process is useful for prepn. of chimera compds. and S-S bond-contg. compds.

IC ICM C07D239-46
ICS C07D473-16; C07D473-18; C07D473-34; C07D487-04; C07H021-00
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 6, 33
IT 25477-96-7P 149411-94-9P 168263-86-3P 171406-46-5P 171486-04-7P 196497-31-1P 196497-32-2P 202343-69-9P 211321-08-3P 211321-09-4P 213552-01-3P 213552-02-4P 213552-03-5P 213552-04-6P 213552-05-7P 213552-06-8P **213552-07-9P 213552-08-0P** 213552-09-1P 213552-13-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of nucleic acid-binding peptides using specific protection/deprotection strategy)
IT **213552-07-9P 213552-08-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of nucleic acid-binding peptides using specific protection/deprotection strategy)
RN 213552-07-9 HCAPLUS
CN 9H-Purine-9-acetic acid, 2,6-bis[(2-methyl-1-oxopropyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)



RN 213552-08-0 HCAPLUS
CN Glycine, N-[[2,6-bis[(2-methyl-1-oxopropyl)amino]-9H-purin-9-yl]acetyl]-N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 6 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:494641 HCAPLUS
DOCUMENT NUMBER: 129:227384
TITLE: Exploiting chemical libraries, structure, and genomics in the search for kinase inhibitors
AUTHOR(S): Gray, Nathanael S.; Wodicka, Lisa; Thunnissen, Andy-Mark W. H.; Norman, Thea C.; Kwon, Soojin; Espinoza, F. Hernan; Morgan, David O.; Barnes, Georjana; LeClerc, Sophie; Meijer, Laurent; Kim, Sung-Hou; Lockhart, David J.; Schultz, Peter G.
CORPORATE SOURCE: Howard Hughes Med. Inst., Univ. California, Berkeley, CA, 94720, USA
SOURCE: Science (Washington, D. C.) (1998), 281(5376), 533-538
CODEN: SCIEAS; ISSN: 0036-8075
PUBLISHER: American Association for the Advancement of Science
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Selective protein kinase inhibitors were developed on the basis of the unexpected binding mode of 2,6,9-trisubstituted purines to the ATP-binding site of the human cyclin-dependent kinase 2 (CDK2). By iterating chem. library synthesis and biol. screening, potent inhibitors of the human CDK2-cyclin A kinase complex and of Saccharomyces cerevisiae Cdc28p were identified. The structural basis for the binding affinity and selectivity was detd. by anal. of a three-dimensional crystal structure of a CDK2-inhibitor complex. The cellular effects of these compds. were characterized in mammalian cells and yeast. In the latter case the effects were characterized on a genome-wide scale by monitoring changes in mRNA levels in treated cells with high-d. oligonucleotide probe arrays. Purine libraries could provide useful tools for analyzing a variety of

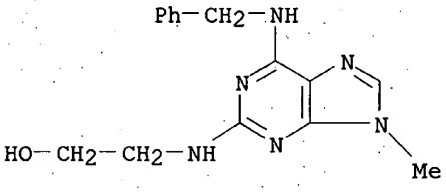
signaling and regulatory pathways and may led to the development of new therapeutics.

CC 7-3 (Enzymes)
Section cross-reference(s): 1, 26, 75

IT **101622-51-9P**, Olomoucine 146426-40-6P, Flavopiridol
186692-46-6P, Roscovitine 212779-48-1P **212779-49-2P**
212844-54-7P, Purvalanol B
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(prepn. and characterization of a combinatorial library of 2,6,9-trisubstituted purine inhibitors of protein kinases)

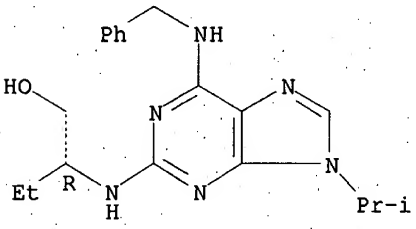
IT **101622-51-9P**, Olomoucine **186692-46-6P**, Roscovitine
212779-49-2P
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)
(prepn. and characterization of a combinatorial library of 2,6,9-trisubstituted purine inhibitors of protein kinases)

RN 101622-51-9 HCAPLUS
CN Ethanol, 2-[[9-methyl-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)

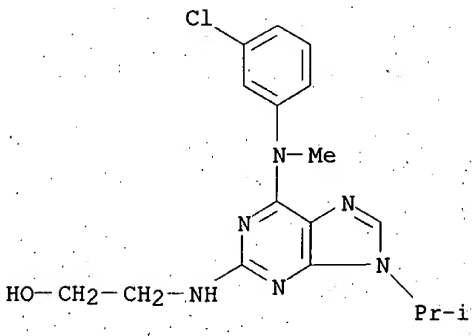


RN 186692-46-6 HCAPLUS
CN 1-Butanol, 2-[[9-(1-methylethyl)-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 212779-49-2 HCAPLUS
CN Ethanol, 2-[[6-[(3-chlorophenyl)methylamino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)

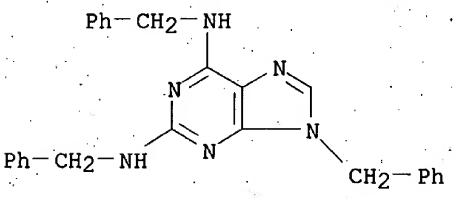


REFERENCE COUNT: 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

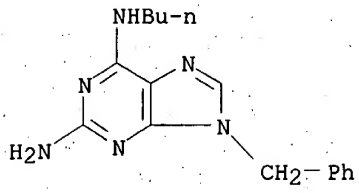
L5 ANSWER 7 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:177003 HCAPLUS
DOCUMENT NUMBER: 128:230182
TITLE: Solution-phase synthesis of 2,6,9-trisubstituted purines
AUTHOR(S): Fiorini, Maria T.; Abell, Chris
CORPORATE SOURCE: University Chemical Laboratory, Cambridge, CB2 IEW, UK
SOURCE: Tetrahedron Letters (1998), 39(13), 1827-1830
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A simple three-step method for the soln.-phase combinatorial synthesis of 2,6,9-trisubstituted purines from 2,6-dichloropurine is described. The synthesis exploits the use of resin capture to remove excess reagent used in the final step.

CC 26-9 (Biomolecules and Their Synthetic Analogs)
IT **204633-53-4P** 204633-54-5P 204633-55-6P 204633-56-7P
204633-57-8P 204633-58-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(soln.-phase synthesis of 2,6,9-trisubstituted purines)
IT **204633-53-4P 204633-57-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(soln.-phase synthesis of 2,6,9-trisubstituted purines)
RN 204633-53-4 HCAPLUS
CN 9H-Purine-2,6-diamine, N,N',9-tris(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 204633-57-8 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-butyl-9-(phenylmethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 8 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:115390 HCAPLUS
DOCUMENT NUMBER: 128:177410
TITLE: Peptide nucleic acids with enhanced solubility having alkylamine side chains
INVENTOR(S): Buchardt, Ole; Egholm, Michael; Nielsen, Peter Eigil; Berg, Rolf Henrik
PATENT ASSIGNEE(S): Den.
SOURCE: U.S., 68 pp. Cont.-in-part of U.S. Ser. No. 108,591. CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5714331 A		19980203	US 1996-686116	19960724
PRIORITY APPLN. INFO.:			DK 1991-986	19910524
			DK 1991-987	19910524
			DK 1992-510	19920415
			US 1993-108591	19931122

OTHER SOURCE(S): MARPAT 128:177410

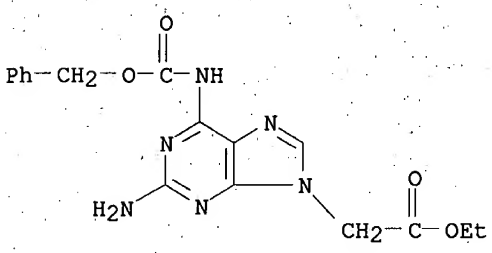
AB The title peptide nucleic acids (PNAs) contain aminoethyl-amino acid backbones in which at least one of the amino acids has a C1-C8 alkylamine side chain, e.g. aminoethyl-D-lysine. The syntheses of many PNA's with aminoethylglycine backbones as well as monomers for these PNA's are presented. Thus, the Tm for PNA H-GTkAGATkCACTk-NH2 (I; aminoethylglycine backbone except where k appears, which is aminoethyl-D-lysine) binding to antiparallel complementary DNA was 55.degree. while that for for PNA H-GTAGATCACT-NH2 (II; with aminoethylglycine backbone) was 52.degree.. The presence of the D-Lys also enhanced sequence specificity: in the presence of a single mismatch in the complementary DNA, the Tm's were 38.degree. and 42.degree. for I and II, resp. A 16-mer PNA contg. four lysine side chains was sol. in physiol. useful solns. while the PNA devoid of the lysine side chains was insol. In in vitro hepatitis C virus mRNA translation assays, a 12-mer PNA contg. two 2,6-diaminopurine nucleobases bearing lysine side chains had an EC50 of .apprx.29nM.

IC C12Q001-68
NCL 435006000
CC 6-2 (General Biochemistry)
Section cross-reference(s): 1
IT 183127-27-7P **202343-70-2P 202343-71-3P**
202999-26-6P 202999-27-7P 203134-29-6P 203265-75-2P
203265-76-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

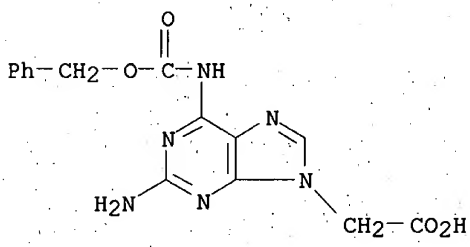
(peptide nucleic acids with enhanced soly. having alkylamine side chains)

IT **202343-70-2P 202343-71-3P 202999-26-6P 202999-27-7P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(peptide nucleic acids with enhanced soly. having alkylamine side chains)

RN 202343-70-2 HCAPLUS
CN 9H-Purine-9-acetic acid, 2-amino-6-[[(phenylmethoxy)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

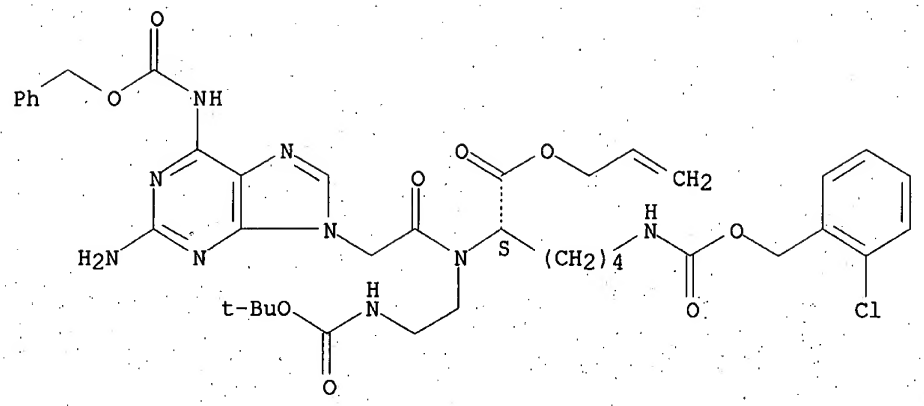


RN 202343-71-3 HCAPLUS
CN 9H-Purine-9-acetic acid, 2-amino-6-[[(phenylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



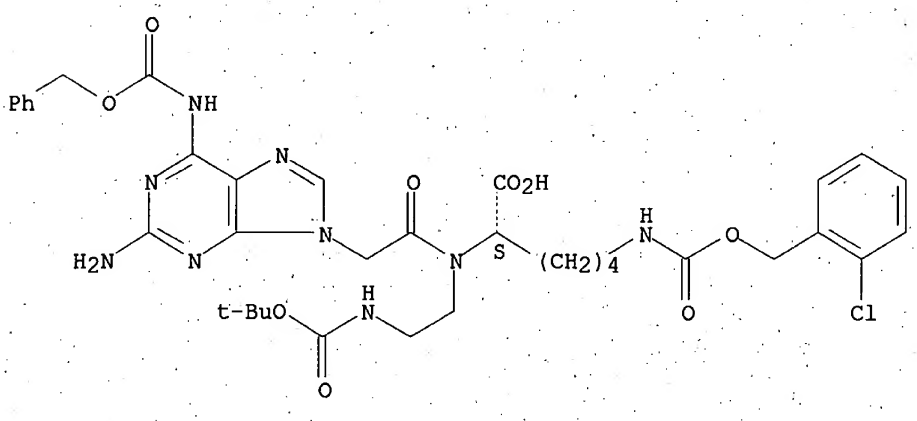
RN 202999-26-6 HCAPLUS
CN 13-Oxa-2,8,11-triazapentadecanoic acid, 8-[[2-amino-6-[[(phenylmethoxy)carbonyl]amino]-9H-purin-9-yl]acetyl]-14,14-dimethyl-12-oxo-7-[(2-propenyloxy)carbonyl]-, (2-chlorophenyl)methyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 202999-27-7 HCAPLUS
CN 13-Oxa-2,8,11-triazapentadecanoic acid, 8-[[2-amino-6-[[(phenylmethoxy)carbonyl]amino]-9H-purin-9-yl]acetyl]-7-carboxy-14,14-dimethyl-12-oxo-, 1-[(2-chlorophenyl)methyl] ester, (S)- (9CI) (CA INDEX NAME)

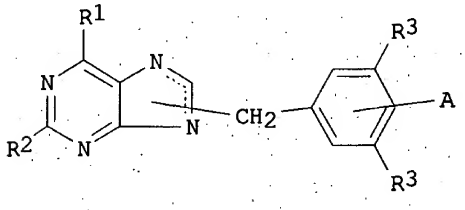
Absolute stereochemistry.



L5 ANSWER 9 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:79439 HCAPLUS
DOCUMENT NUMBER: 128:180423
TITLE: Preparation and formulation of purine derivatives as antitumor agents
INVENTOR(S): Matsuda, Akira; Sasaki, Takuma; Shuto, Akira; Uemoto, Kazuhiro
PATENT ASSIGNEE(S): Matsuda, Akira, Japan; Sasaki, Takuma; Toa Eiyo, Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 37 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10025294	A2	19980127	JP 1997-88702	19970325

PRIORITY APPLN. INFO.: JP 1996-94673 19960326
OTHER SOURCE(S): MARPAT 128:180423
GI



I

AB The title compds. I [R1 = H, halo, etc.; R2 = H, amino; R3 = H, halo; A = H, halo, alkyl, etc.] are prepd. 2-Amino-6-chloro-9-[4-(phenylmethyl)benzyl]-9H-purine (II) in vitro showed IC50 of 0.3 .mu.g/mL against NIH3T3-Ha-ras cells (cells with Ha-ras gene). II in vitro showed IC50 of > 50 .mu.g/mL against normal NIH3T3 cells. L-651 582, an antitumor agent currently in clin. trial, in vitro showed IC50 of 5.56 .mu.g/mL against NIH3T3-Ha-ras cells. The angiogenesis inhibiting activities of I are more potent than that of L-651 582.

IC ICM C07D473-40
ICS A61K031-52; C07D473-30; C07D473-34; C07D473-38

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

IT 101134-10-5P 101134-11-6P 117860-38-5P 203201-57-4P 203201-58-5P
203201-59-6P 203201-60-9P 203201-61-0P 203201-62-1P 203201-63-2P
203201-64-3P 203201-65-4P 203201-66-5P 203201-67-6P 203201-68-7P
203201-69-8P 203201-70-1P 203201-71-2P 203201-72-3P 203201-73-4P
203201-74-5P 203201-75-6P 203201-76-7P 203201-77-8P 203201-78-9P
203201-79-0P 203201-80-3P 203201-81-4P 203201-82-5P 203201-83-6P
203201-84-7P 203201-85-8P 203201-86-9P 203201-87-0P 203201-88-1P
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203201-94-9P 203201-95-0P 203201-96-1P 203201-97-2P 203201-98-3P
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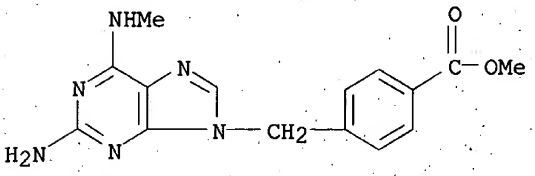
203202-08-8P 203202-10-2P 203202-12-4P 203202-14-6P
203202-15-7P 203202-16-8P 203202-17-9P 203202-18-0P 203202-19-1P
203202-20-4P 203202-21-5P 203202-22-6P 203202-23-7P 203202-24-8P
203202-25-9P 203202-26-0P 203202-27-1P 203202-28-2P 203202-29-3P
203202-30-6P 203202-31-7P 203202-32-8P 203202-33-9P 203202-34-0P
203202-35-1P 203202-36-2P 203202-37-3P 203202-38-4P 203202-39-5P
203202-40-8P 203202-41-9P 203202-42-0P 203202-43-1P 203202-44-2P
203202-45-3P 203202-46-4P 203202-47-5P 203202-48-6P 203202-50-0P
203202-51-1P 203202-52-2P 203202-53-3P 203202-54-4P 203202-55-5P
203202-56-6P 203202-57-7P 203202-58-8P 203202-59-9P 203202-60-2P
203202-61-3P 203202-62-4P 203202-63-5P 203202-64-6P 203202-65-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of purine derivs. as antitumor agents)

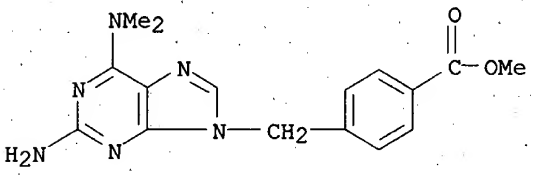
IT **203202-08-8P 203202-10-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of purine derivs. as antitumor agents)

RN 203202-08-8 HCAPLUS
CN Benzoic acid, 4-[[2-amino-6-(methylamino)-9H-purin-9-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)



RN 203202-10-2 HCAPLUS
CN Benzoic acid, 4-[[2-amino-6-(dimethylamino)-9H-purin-9-yl]methyl]-, methyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 10 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:15082 HCAPLUS
DOCUMENT NUMBER: 128:150720
TITLE: Increased DNA binding and sequence discrimination of PNA oligomers containing 2,6-diaminopurine
AUTHOR(S): Haaiima, Gerald; Hansen, Henrik F.; Christensen, Leif; Dahl, Otto; Nielsen, Peter E.
CORPORATE SOURCE: Center for Biomolecular Recognition, Department of Chemistry, The H.C. Orsted Institute, Universitetsparken 5, Copenhagen, DK-2100, Den.
SOURCE: Nucleic Acids Research (1997), 25(22), 4639-4643
CODEN: NARHAD; ISSN: 0305-1048
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:150720

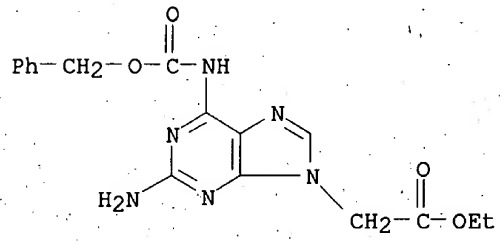
AB The synthesis of a diaminopurine PNA monomer, N-[N6-(benzyloxycarbonyl)-2,6-diaminopurine-9-yl] acetyl-N(2-t-butyloxycarbonylaminoethyl)glycine, and the incorporation of this monomer into PNA oligomers are described. Substitution of adenine by diaminopurine in PNA oligomers increased the Tm of duplexes formed with complementary DNA, RNA or PNA by 2.5-6.5.degree.C per diaminopurine. Furthermore, discrimination against mismatches facing the diaminopurine in the hybridizing oligomer is improved. Finally, a homopurine decamer PNA contg. six diaminopurines is shown to form a (gel shift) stable strand displacement complex with a target in a 246 bp double-stranded DNA fragment.

CC 6-2 (General Biochemistry)
Section cross-reference(s): 3, 34

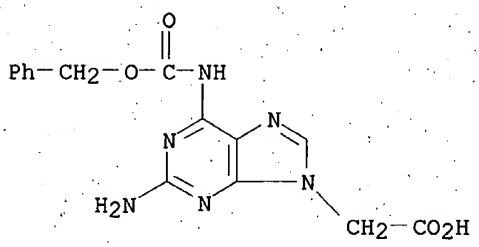
IT 202343-69-9P **202343-70-2P 202343-71-3P**
202343-72-4P 202343-73-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(increased DNA binding and sequence discrimination of PNA oligomers contg. 2,6-diaminopurine)

IT **202343-70-2P 202343-71-3P 202343-72-4P**
202343-73-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(increased DNA binding and sequence discrimination of PNA oligomers contg. 2,6-diaminopurine)

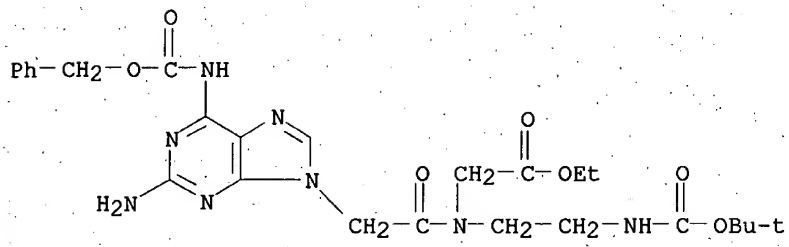
RN 202343-70-2 HCAPLUS
CN 9H-Purine-9-acetic acid, 2-amino-6-[[(phenylmethoxy)carbonyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)



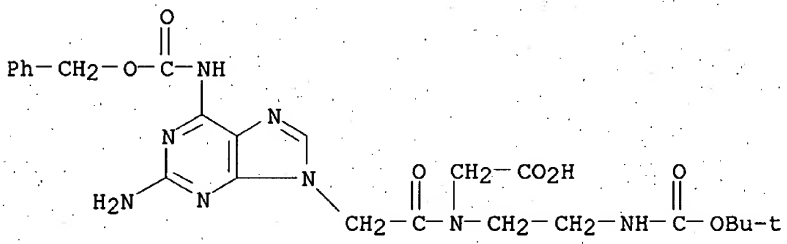
RN 202343-71-3 HCAPLUS
CN 9H-Purine-9-acetic acid, 2-amino-6-[[(phenylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 202343-72-4 HCAPLUS
CN Glycine, N-[[2-amino-6-[[(phenylmethoxy)carbonyl]amino]-9H-purin-9-yl]acetyl]-N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 202343-73-5 HCAPLUS
CN Glycine, N-[[2-amino-6-[[(phenylmethoxy)carbonyl]amino]-9H-purin-9-yl]acetyl]-N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]- (9CI) (CA INDEX NAME)

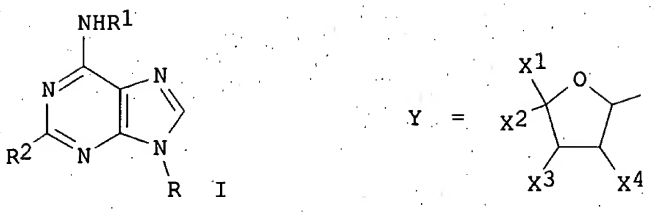


REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 11 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:761605 HCAPLUS
DOCUMENT NUMBER: 128:34983
TITLE: Preparation of nucleosides as A3 adenosine receptor agonists
INVENTOR(S): Jacobson, Kenneth A.; Jeong, Heaok Kim; Siddiqi, Suhaib M.; Johnson, Carl R.; Secrist, John A., III; Tiwari, Kamal N.
PATENT ASSIGNEE(S): United States Dept. of Health and Human Services, USA
SOURCE: U.S., 35 pp., Cont.-in-part of U.S. Ser. No. 274,628.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5688774	A	19971118	US 1995-396111	19950228
US 5773423	A	19980630	US 1994-274628	19940713

PRIORITY APPLN. INFO.: US 1993-91109 B2 19930713
US 1993-163324 B2 19931206
US 1994-274628 A2 19940713
OTHER SOURCE(S): MARPAT 128:34983
GI



AB Title nucleosides I (R = H, Y; R1 = benzyl, halobenzyl; R2 = H, halo, alkylamino; X1 = H, alkyl; X2 = alkylamido; X3, X4 = independently H, OH, NH2, N3, halo, Bz) were prepd. as A3 adenosine receptor agonists. The present invention also provides a method of selectively activating an A3 adenosine receptor in a mammal, which method comprises acutely or chronically administering to a mammal in need of selective activation of its A3 adenosine receptor a therapeutically or prophylactically effective amt. of a compd. which binds with the A3 receptor so as to stimulate an A3 receptor-dependent response. Thus, N3-(3-iodobenzyl)-9-Me adenine was prepd. and showed an affinity at rat brain adenosine receptors (Ki = 2.23-48.3 .mu.M).

IC ICM A61K031-70
ICS C07H019-167; C07H019-173

NCL 514046000

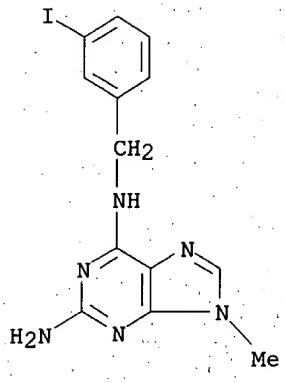
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63

IT 163042-60-2P 163042-61-3P 163042-62-4P 163042-63-5P 163042-64-6P
163042-65-7P 163042-66-8P **163042-67-9P** 163042-68-0P
163042-69-1P 163042-70-4P 163042-71-5P
163042-72-6P 163042-73-7P 163042-74-8P 163042-75-9P
163042-78-2P 163042-79-3P 163042-81-7P 163042-83-9P 163042-84-0P
163042-88-4P 163042-89-5P 170966-22-0P 170966-23-1P 170966-25-3P
199473-26-2P 199473-29-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of nucleosides as a adenosine receptor agonists)

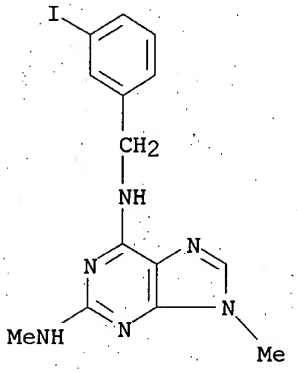
IT **163042-67-9P 163042-69-1P 163042-70-4P**
163042-71-5P 163042-72-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of nucleosides as a adenosine receptor agonists)

RN 163042-67-9 HCAPLUS

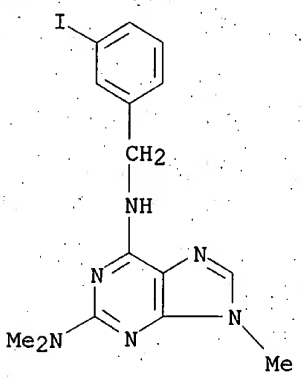
CN 9H-Purine-2,6-diamine, N6-[(3-iodophenyl)methyl]-9-methyl- (9CI) (CA INDEX NAME)



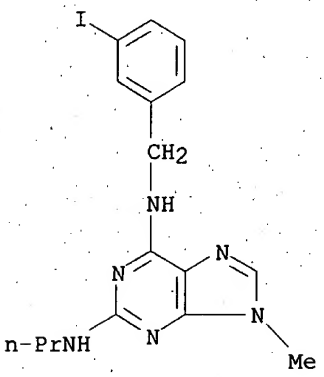
RN 163042-69-1 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(3-iodophenyl)methyl]-N2,9-dimethyl- (9CI) (CA INDEX NAME)



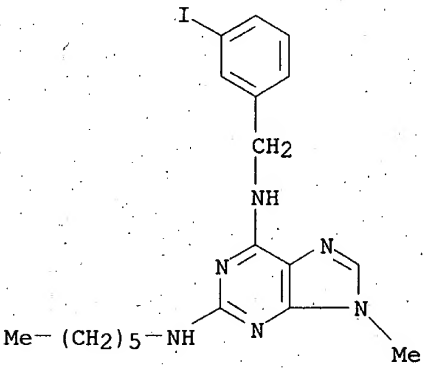
RN 163042-70-4 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(3-iodophenyl)methyl]-N2,N2,9-trimethyl- (9CI) (CA INDEX NAME)



RN 163042-71-5 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(3-iodophenyl)methyl]-9-methyl-N2-propyl- (9CI) (CA INDEX NAME)



RN 163042-72-6 HCAPLUS
CN 9H-Purine-2,6-diamine, N2-hexyl-N6-[(3-iodophenyl)methyl]-9-methyl- (9CI) (CA INDEX NAME)



L5 ANSWER 12 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:741197 HCAPLUS
DOCUMENT NUMBER: 128:48081
TITLE: Synthesis and activity of 2,6,9-trisubstituted purines
AUTHOR(S): Schow, Steven R.; Mackman, Richard L.; Blum, Cheri L.; Brooks, Eric; Horsma, Amy G.; Joly, Alison; Kerwar, Suresh S.; Lee, Gavin; Shiffman, Dov; Nelson, Marek G.; Wang, Xingbo; Wick, Michael M.; Zhang, Xiaoming; Lum, Robert T.
CORPORATE SOURCE: CV Therapeutics, Inc., Palo Alto, CA, 94304, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1997), 7(21), 2697-2702
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal
LANGUAGE: English

AB The prepn. of a series of 2,6,9-trisubstituted purines and the structure-activity data for the inhibition of cyclin dependent kinase, CDK2 are presented. 2,6-Dichloropurine was treated with a primary amine or aniline to displace the 6-chloro group followed by addn. of an alkyl halide to provide alkylation at the 9 position. No 7 alkylation was obsd. Displacement of the 2-chloro was the most difficult requiring 1:1 mixt. of N-methylpyrrolidinone and amine at 135.cntdot. for 24-40 h.

CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1, 3, 7

IT **101622-51-9,** Olomoucine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(prepn. of 2,6,9-trisubstituted purines and their structure-activity data for the inhibition of cyclin dependent kinase)

IT 1681-15-8DP, derivs. 39639-47-9P 135394-16-0P 199986-70-4P
199986-71-5P 199986-72-6P **199986-74-8P**
199986-75-9P 199986-76-0P **199986-79-3P** 199986-82-8P
199986-85-1P **199986-88-4P** **199986-90-8P**
199986-92-0P 199986-95-3P **199986-96-4P**
199986-98-6P 199987-00-3P **199987-02-5P** 199987-05-8P
199987-07-0P 199987-08-1P **199987-11-6P**
199987-12-7P **199987-14-9P** 199987-16-1P
199987-19-4P **199987-21-8P** 199987-25-2P 199987-28-5P
199987-30-9P **199987-32-1P** **199987-34-3P**
199987-36-5P 199987-39-8P **199987-42-3P** 199987-43-4P
199987-45-6P **199987-47-8P** **199987-49-0P**
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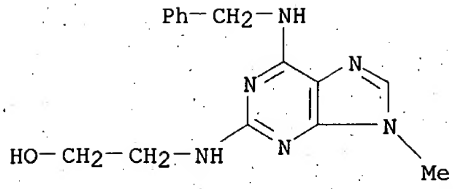
199987-89-8P 199987-91-2P 199987-94-5P 199987-96-7P 199987-98-9P
199988-00-6P 199988-02-8P 199988-04-0P **199988-06-2P**
199988-08-4P **199988-11-9P** **199988-13-1P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of 2,6,9-trisubstituted purines and their structure-activity data for the inhibition of cyclin dependent kinase)

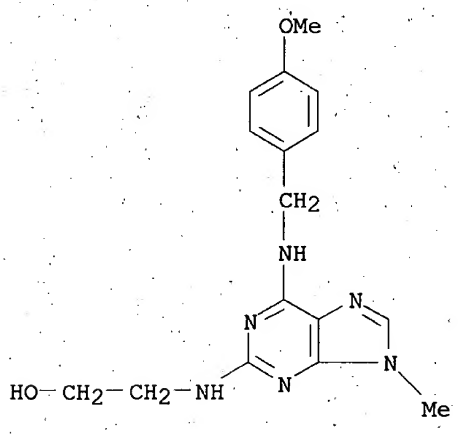
IT **101622-51-9,** Olomoucine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(prepn. of 2,6,9-trisubstituted purines and their structure-activity data for the inhibition of cyclin dependent kinase)

RN 101622-51-9 HCAPLUS
CN Ethanol, 2-[[9-methyl-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)

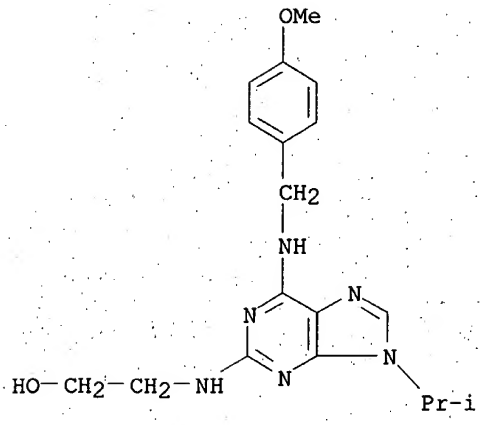


IT **199986-71-5P 199986-74-8P 199986-75-9P**
199986-79-3P 199986-88-4P 199986-90-8P
199986-92-0P 199986-96-4P 199986-98-6P
199987-02-5P 199987-07-0P 199987-11-6P
199987-12-7P 199987-14-9P 199987-19-4P
199987-21-8P 199987-32-1P 199987-34-3P
199987-36-5P 199987-42-3P 199987-45-6P
199987-47-8P 199987-49-0P 199987-51-4P
199987-57-0P 199987-60-5P 199987-63-8P
199987-65-0P 199987-67-2P 199987-69-4P
199987-71-8P 199987-77-4P 199987-81-0P
199988-06-2P 199988-11-9P 199988-13-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. of 2,6,9-trisubstituted purines and their structure-activity data for the inhibition of cyclin dependent kinase)

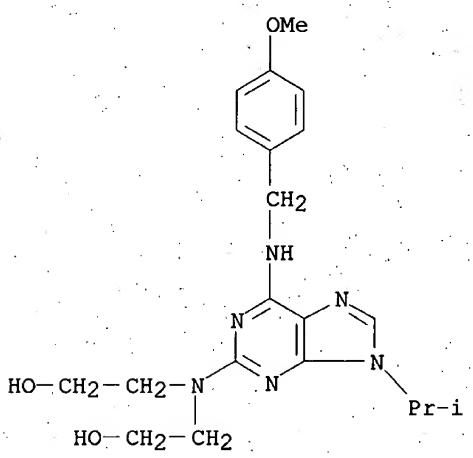
RN 199986-71-5 HCAPLUS
CN Ethanol, 2-[[6-[[(4-methoxyphenyl)methyl]amino]-9-methyl-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



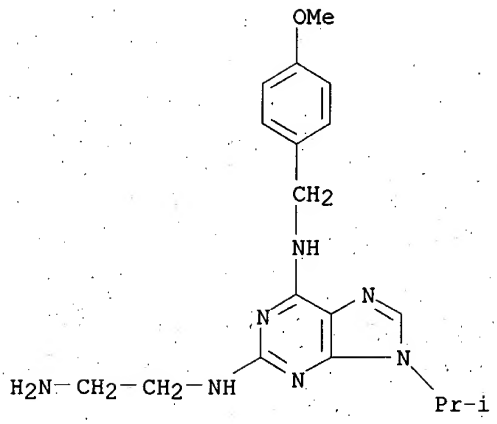
RN 199986-74-8 HCAPLUS
CN Ethanol, 2-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



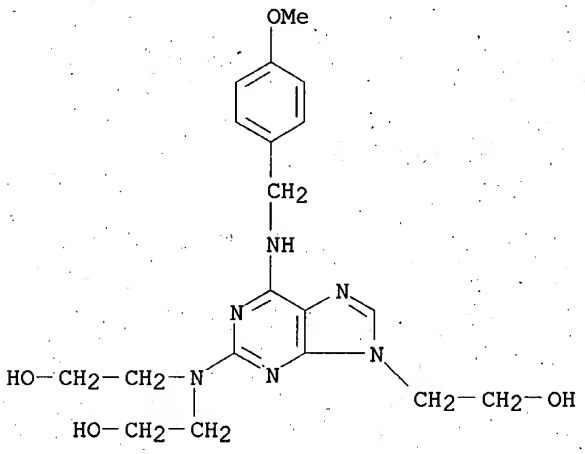
RN 199986-75-9 HCAPLUS
CN Ethanol, 2,2'-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



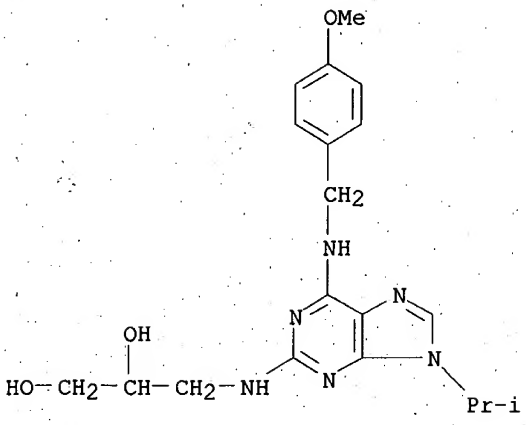
RN 199986-79-3 HCAPLUS
CN 9H-Purine-2,6-diamine, N2-(2-aminoethyl)-N6-[(4-methoxyphenyl)methyl]-9-(1-methylethyl)- (9CI) (CA INDEX NAME)



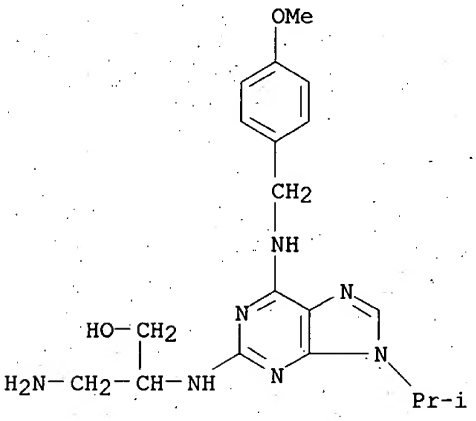
RN 199986-88-4 HCAPLUS
CN 9H-Purine-9-ethanol, 2-[bis(2-hydroxyethyl)amino]-6-[[(4-methoxyphenyl)methyl]amino]- (9CI) (CA INDEX NAME)



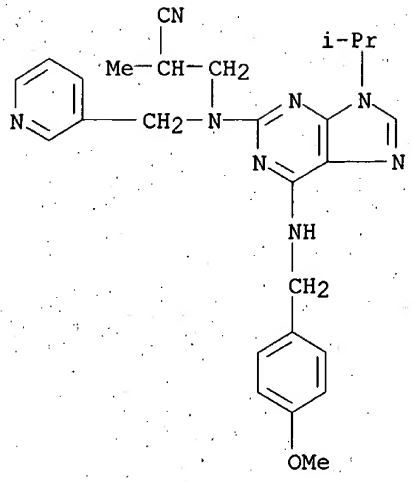
RN 199986-90-8 HCAPLUS
CN 1,2-Propanediol, 3-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



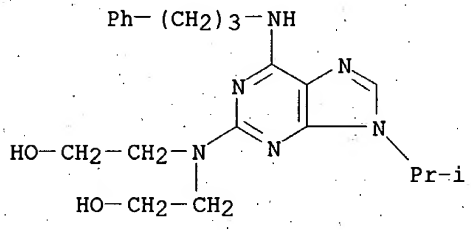
RN 199986-92-0 HCAPLUS
CN 1-Propanol, 3-amino-2-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



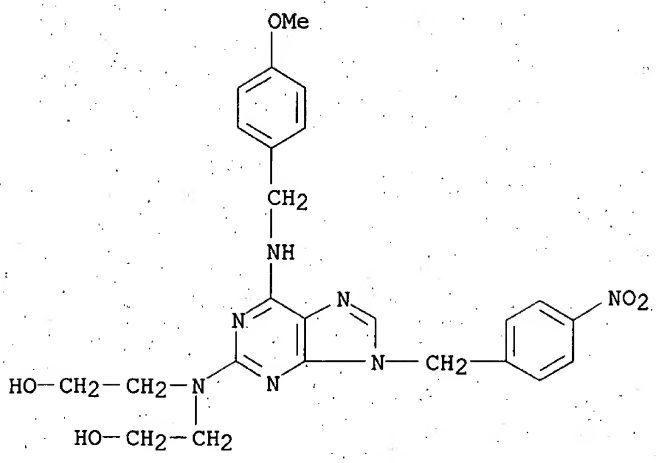
RN 199986-96-4 HCAPLUS
CN Propanenitrile, 3-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl](3-pyridinylmethyl)amino]-2-methyl- (9CI) (CA INDEX NAME)



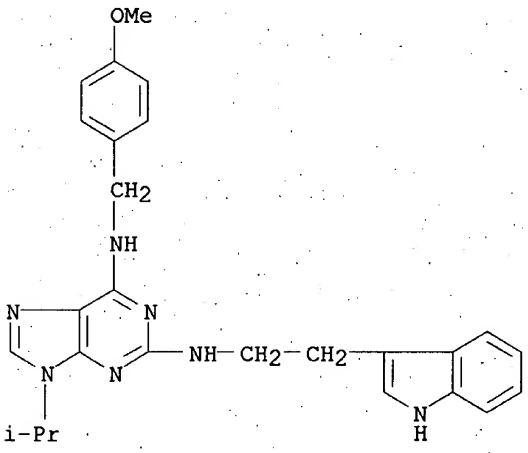
RN 199986-98-6 HCAPLUS
CN Ethanol, 2,2'-[[9-(1-methylethyl)-6-[(3-phenylpropyl)amino]-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



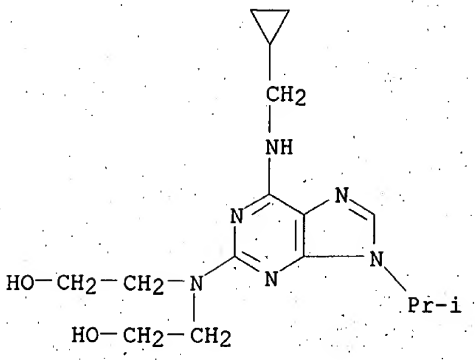
RN 199987-02-5 HCAPLUS
CN Ethanol, 2,2'-[[6-[[(4-methoxyphenyl)methyl]amino]-9-[(4-nitrophenyl)methyl]-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



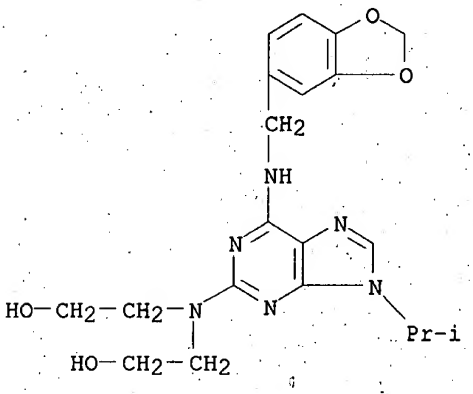
RN 199987-07-0 HCAPLUS
CN 9H-Purine-2,6-diamine, N2-[2-(1H-indol-3-yl)ethyl]-N6-[(4-methoxyphenyl)methyl]-9-(1-methylethyl)- (9CI) (CA INDEX NAME)



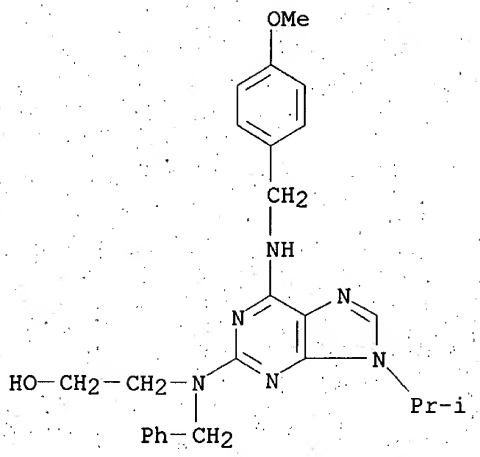
RN 199987-11-6 HCAPLUS
CN Ethanol, 2,2'-[[6-[(cyclopropylmethyl)amino]-9-(1-methylethyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



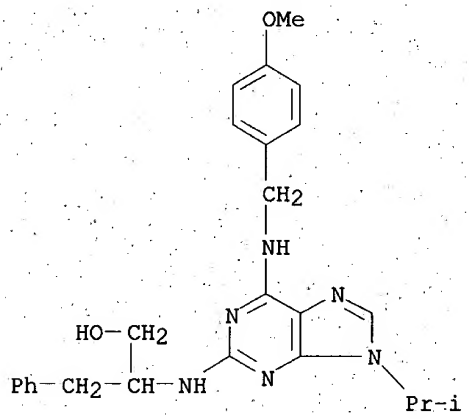
RN 199987-12-7 HCAPLUS
CN Ethanol, 2,2'-[[6-[(1,3-benzodioxol-5-ylmethyl)amino]-9-(1-methylethyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



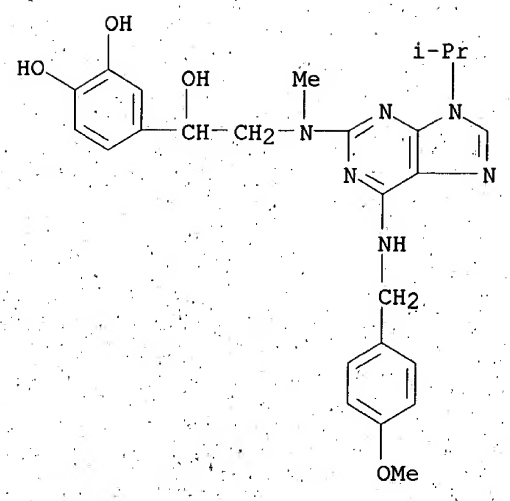
RN 199987-14-9 HCAPLUS
CN Ethanol, 2-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl](phenylmethyl)amino]- (9CI) (CA INDEX NAME)



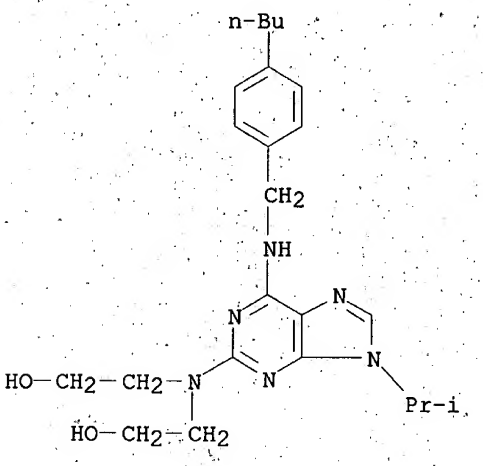
RN 199987-19-4 HCAPLUS
CN Benzenepropanol, .beta.-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



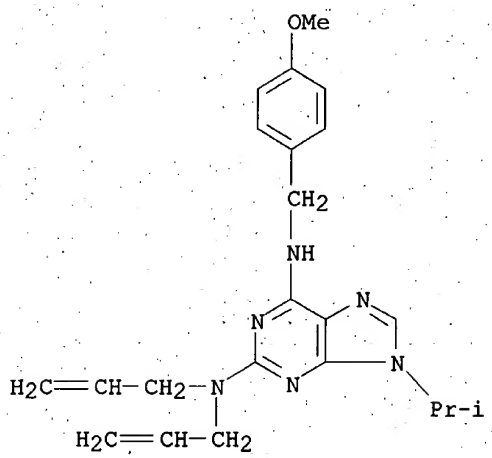
RN 199987-21-8 HCAPLUS
CN 1,2-Benzenediol, 4-[1-hydroxy-2-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]methylamino]ethyl]- (9CI) (CA INDEX NAME)



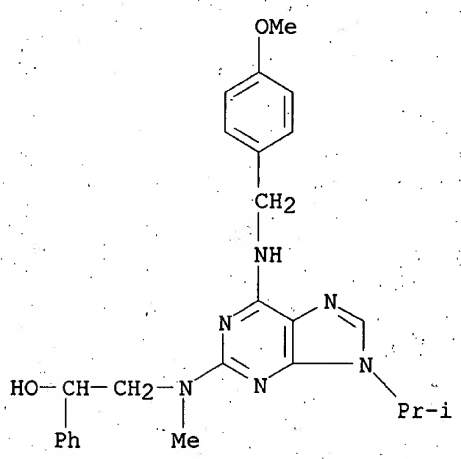
RN 199987-32-1 HCAPLUS
CN Ethanol, 2,2'-[[6-[[(4-butylphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



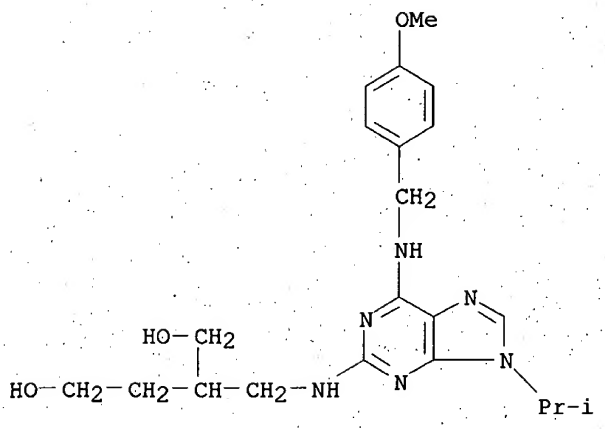
RN 199987-34-3 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(4-methoxyphenyl)methyl]-9-(1-methylethyl)-N2,N2-di-2-propenyl- (9CI) (CA INDEX NAME)



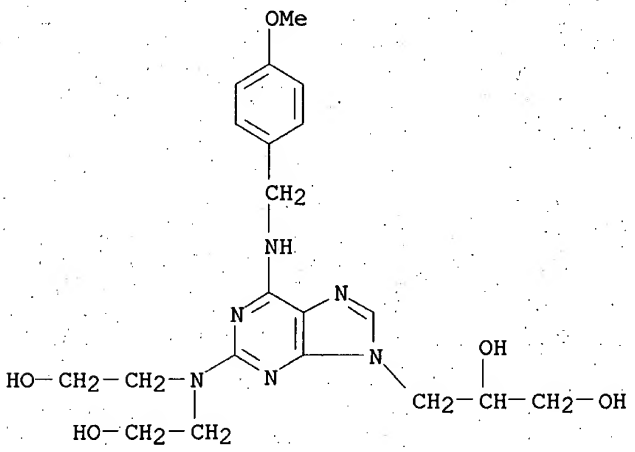
RN 199987-36-5 HCAPLUS
CN Benzenemethanol, .alpha.-[[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]methylamino]methyl]- (9CI) (CA INDEX NAME)



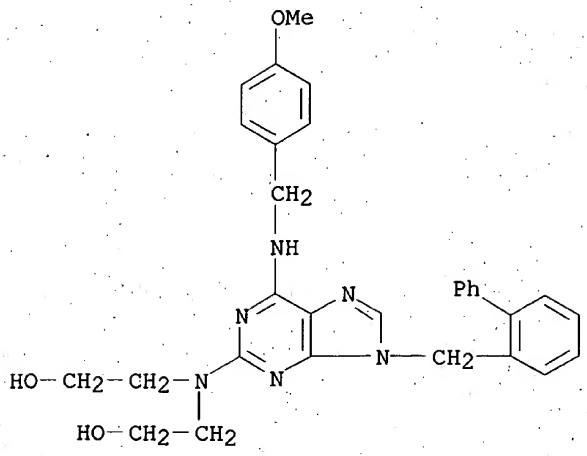
RN 199987-42-3 HCAPLUS
CN 1,4-Butanediol, 2-[[[6-[[(4-methoxyphenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]methyl]- (9CI) (CA INDEX NAME)



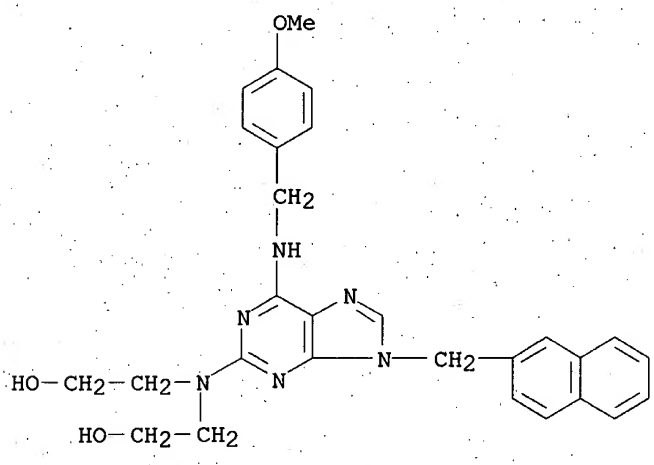
RN 199987-45-6 HCAPLUS
CN 1,2-Propanediol, 3-[2-[bis(2-hydroxyethyl)amino]-6-[[(4-methoxyphenyl)methyl]amino]-9H-purin-9-yl]- (9CI) (CA INDEX NAME)



RN 199987-47-8 HCAPLUS
CN Ethanol, 2,2'-[[9-([1,1'-biphenyl]-2-ylmethyl)-6-[[(4-methoxyphenyl)methyl]amino]-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)

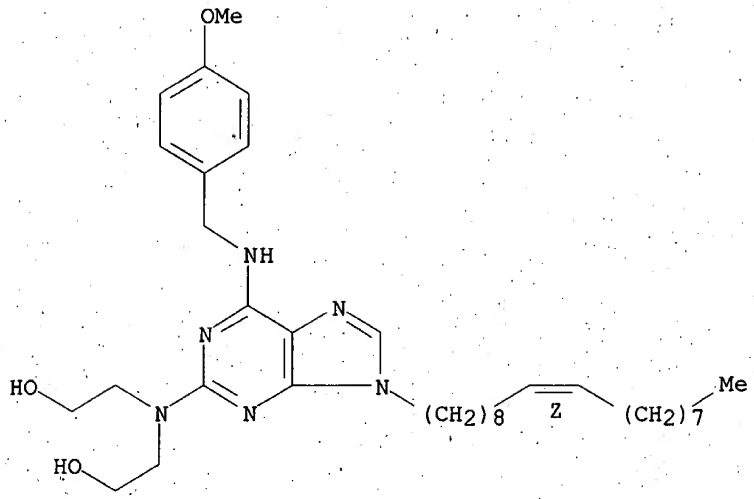


RN 199987-49-0 HCAPLUS
CN Ethanol, 2,2'-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(2-naphthalenylmethyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)

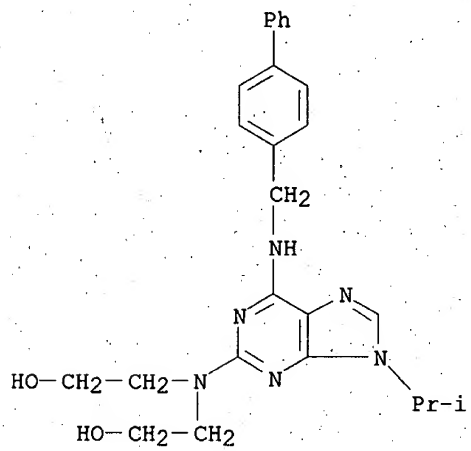


RN 199987-51-4 HCAPLUS
CN Ethanol, 2,2'-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(9Z)-9-octadecenyl-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)

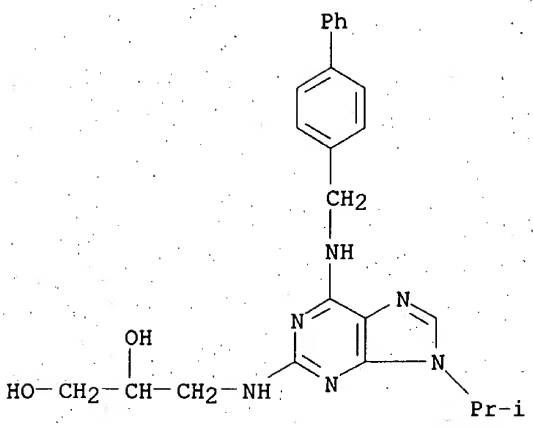
Double bond geometry as shown.



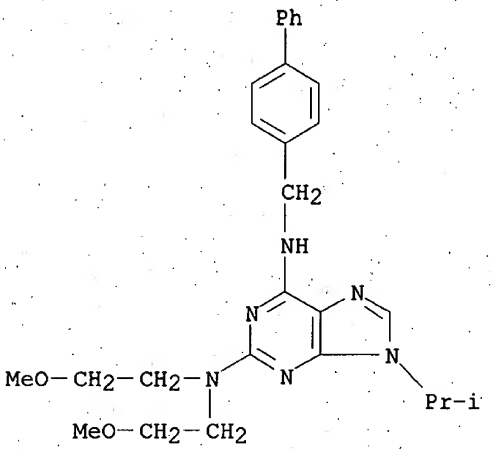
RN 199987-57-0 HCAPLUS
CN Ethanol, 2,2'-[[6-[([1,1'-biphenyl]-4-ylmethyl)amino]-9-(1-methylethyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



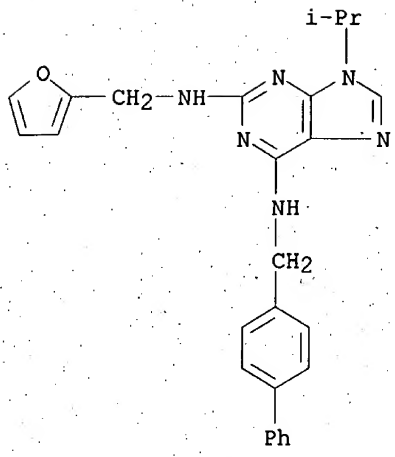
RN 199987-60-5 HCAPLUS
CN 1,2-Propanediol, 3-[[6-[([1,1'-biphenyl]-4-ylmethyl)amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



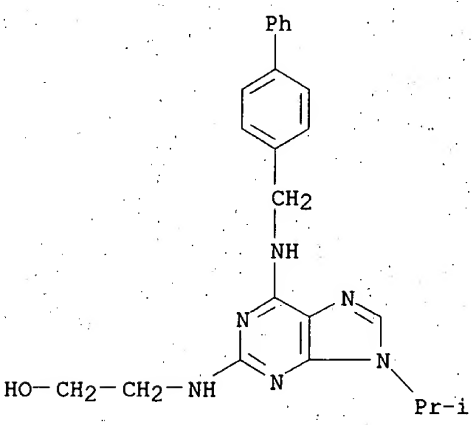
RN 199987-63-8 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-([1,1'-biphenyl]-4-ylmethyl)-N2,N2-bis(2-methoxyethyl)-9-(1-methylethyl)- (9CI) (CA INDEX NAME)



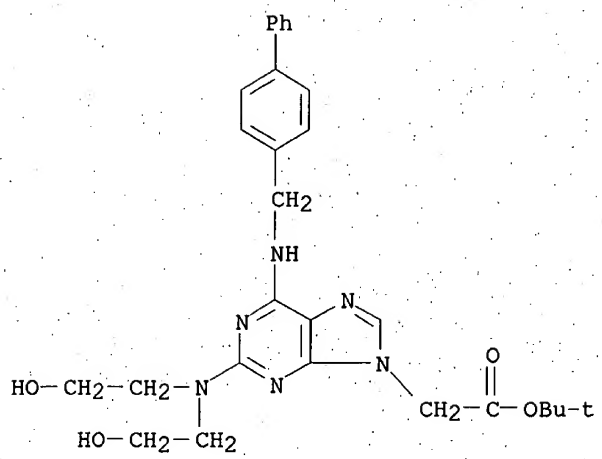
RN 199987-65-0 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-([1,1'-biphenyl]-4-ylmethyl)-N2-(2-furanylmethyl)-9-(1-methylethyl)- (9CI) (CA INDEX NAME)



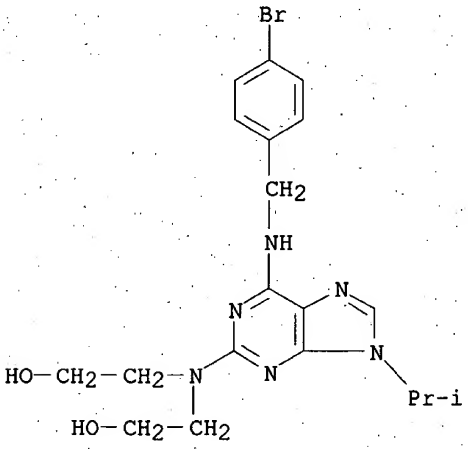
RN 199987-67-2 HCAPLUS
CN Ethanol, 2-[[6-[([1,1'-biphenyl]-4-ylmethyl)amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



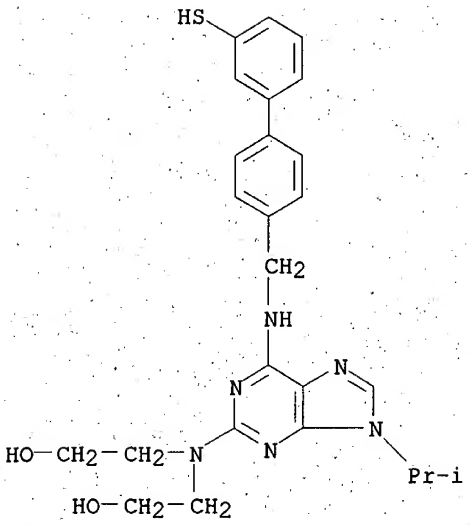
RN 199987-69-4 HCAPLUS
CN 9H-Purine-9-acetic acid, 6-[([1,1'-biphenyl]-4-ylmethyl)amino]-2-[bis(2-hydroxyethyl)amino]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



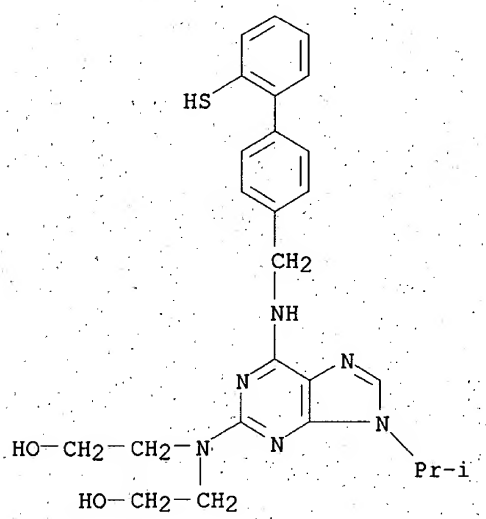
RN 199987-71-8 HCAPLUS
CN Ethanol, 2,2'-[[6-[[(4-bromophenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



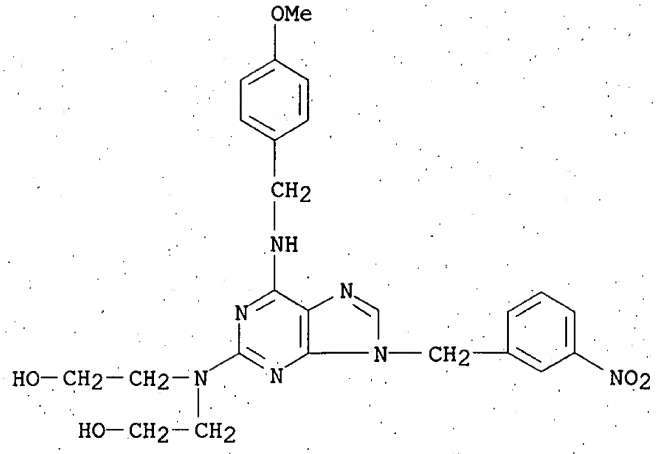
RN 199987-77-4 HCAPLUS
CN Ethanol, 2,2'-[[6-[[(3'-mercapto[1,1'-biphenyl]-4-yl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



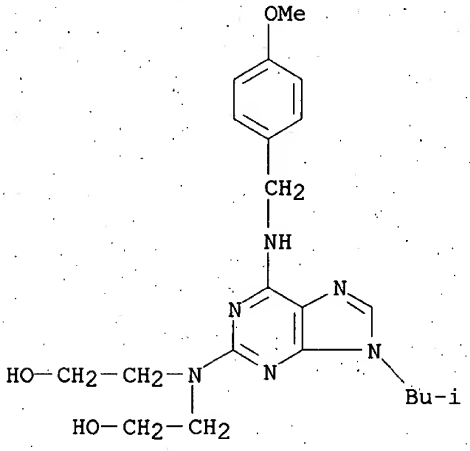
RN 199987-81-0 HCAPLUS
CN Ethanol, 2,2'-[[6-[[(2'-mercapto[1,1'-biphenyl]-4-yl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



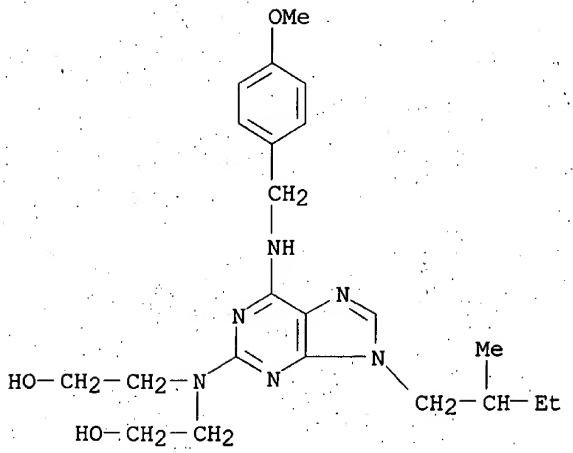
RN 199988-06-2 HCAPLUS
CN Ethanol, 2,2'-[[6-[[(4-methoxyphenyl)methyl]amino]-9-[(3-nitrophenyl)methyl]-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



RN 199988-11-9 HCAPLUS
CN Ethanol, 2,2'-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(2-methylpropyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)



RN 199988-13-1 HCAPLUS
CN Ethanol, 2,2'-[[6-[[(4-methoxyphenyl)methyl]amino]-9-(2-methylbutyl)-9H-purin-2-yl]imino]bis- (9CI) (CA INDEX NAME)

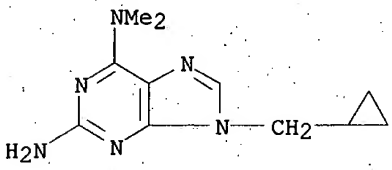


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 13 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:603431 HCAPLUS
DOCUMENT NUMBER: 127:248069
TITLE: 6-(Alkylamino)-9-alkylpurines. A New Class of Potential Antipsychotic Agents
AUTHOR(S): Kelley, James L.; Bullock, R. Morris; Krochmal, Mark P.; McLean, Ed W.; Linn, James A.; Durcan, Micheal J.; Cooper, Barrett R.
CORPORATE SOURCE: Division of Organic Chemistry, Burroughs Wellcome Co., Research Triangle Park, NC, 27709, USA
SOURCE: Journal of Medicinal Chemistry (1997), 40(20), 3207-3216
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of 6-(alkylamino)-9-alkylpurines was synthesized and evaluated for the property of antagonizing the behavioral effects in animals of the dopamine agonist apomorphine. This model for identifying potential antipsychotic agents is based on the hypothesis that agents that antagonize apomorphine-induced aggressive behavior in rats and apomorphine-induced climbing in mice, but that do not block stereotyped behavior, could have an antipsychotic effect in humans without producing extrapyramidal side effects. The antiaggressive-behavior activity of the lead compd. [6-(dimethylamino)-9-(3-phenylalaninamidobenzyl)-9H-purine] was improved 48-fold with 6-(cyclopropylamino)-9-(cyclopropylmethyl)-2-(trifluoromethyl)-9H-purine (80) (po ED50 of 2 mg/kg), which was obtained through an iterative sequence of structure-activity relationship studies that encompassed evaluation of the effects of structure variations at the purine 9-, 6-, and 2-positions. Potency was enhanced with a 9-cyclopropyl group, the duration of action was improved with the 6-(cyclopropylamino) substituent, potency was further enhanced with an N-formyl prodrug, and an agent with reduced cardiovascular effect emerged with the 2-trifluoromethyl purine 80. This potential antipsychotic agent was not developed further due to undesirable effects on the stomach.

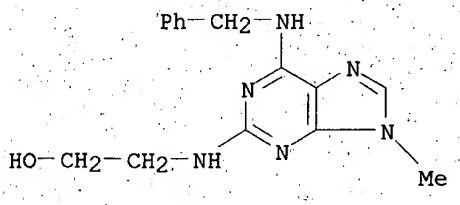
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
IT **195252-71-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and antagonism of apomorphine-induced aggression of aminopurines)
IT **195252-71-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and antagonism of apomorphine-induced aggression of aminopurines)
RN 195252-71-2 HCAPLUS
CN 9H-Purine-2,6-diamine, 9-(cyclopropylmethyl)-N6,N6-dimethyl- (9CI) (CA INDEX NAME)



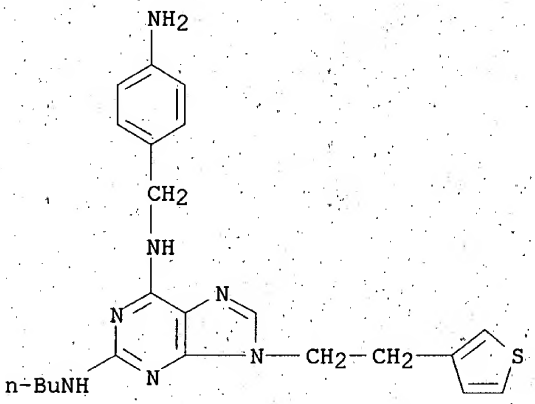
L5 ANSWER 14 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:142821 HCAPLUS
DOCUMENT NUMBER: 126:251019
TITLE: Combinatorial synthesis of 2,9-substituted purines
AUTHOR(S): Gray, Nathanael S.; Kwon, Soojin; Schultz, Peter G.
CORPORATE SOURCE: Howard Hughes Medical Institute, Department of Chemistry, University of California, Berkeley, CA, 94720, USA
SOURCE: Tetrahedron Letters (1997), 38(7), 1161-1164
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A method for the combinatorial synthesis of 2,9-disubstituted purines using a Mitsunobu reaction to alkylate the N-9 position and an amination reaction to install amines at the C-2 position has been developed.
CC 26-9 (Biomolecules and Their Synthetic Analogs)
IT **101622-51-9DP**, Olomoucine, analogs 188644-34-0DP, resin-bound 188644-36-2DP, resin-bound 188644-37-3DP, resin-bound 188644-41-9DP, resin-bound 188644-42-0DP, resin-bound 188644-43-1DP, resin-bound **188644-44-2P 188644-45-3P 188644-46-4P 188644-47-5P 188644-48-6P 188644-49-7P 188644-50-0P** 188644-51-1P 188644-52-2P 188644-53-3P 188644-54-4P 188644-55-5P 188644-56-6P 188644-57-7P 188644-58-8P 188644-59-9P 188644-60-2P 188644-61-3P **188644-62-4P 188644-63-5P 188644-64-6P 188644-65-7P 188644-66-8P 188644-67-9P 188644-68-0P** 188644-69-1P **188644-70-4P 188644-71-5P 188644-72-6P 188644-73-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(combinatorial synthesis of 2,9-diaminopurines)
IT **101622-51-9DP**, Olomoucine, analogs **188644-44-2P 188644-45-3P 188644-46-4P 188644-47-5P 188644-48-6P 188644-49-7P 188644-50-0P**

188644-62-4P 188644-63-5P 188644-64-6P
188644-65-7P 188644-66-8P 188644-67-9P
188644-68-0P 188644-70-4P 188644-71-5P
188644-72-6P 188644-73-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(combinatorial synthesis of 2,9-diaminopurines)

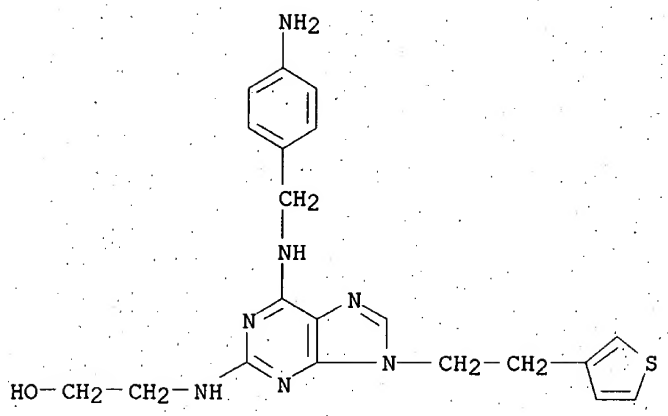
RN 101622-51-9 HCAPLUS
CN Ethanol, 2-[[9-methyl-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



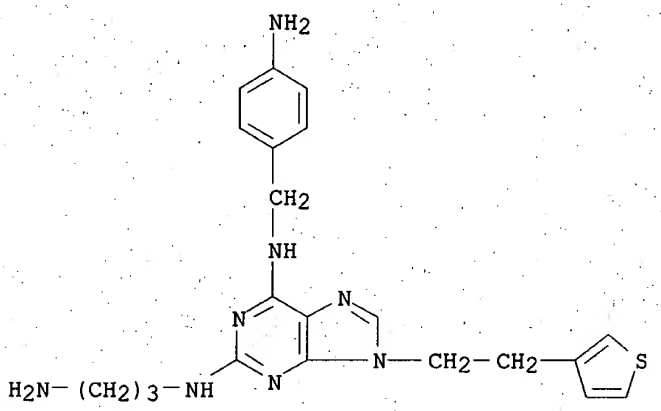
RN 188644-44-2 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(4-aminophenyl)methyl]-N2-butyl-9-[2-(3-thienyl)ethyl]- (9CI) (CA INDEX NAME)



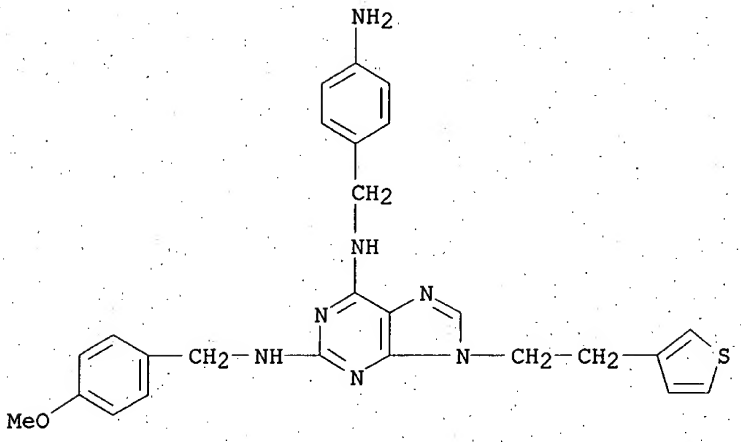
RN 188644-45-3 HCAPLUS
CN Ethanol, 2-[[6-[[(4-aminophenyl)methyl]amino]-9-[2-(3-thienyl)ethyl]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



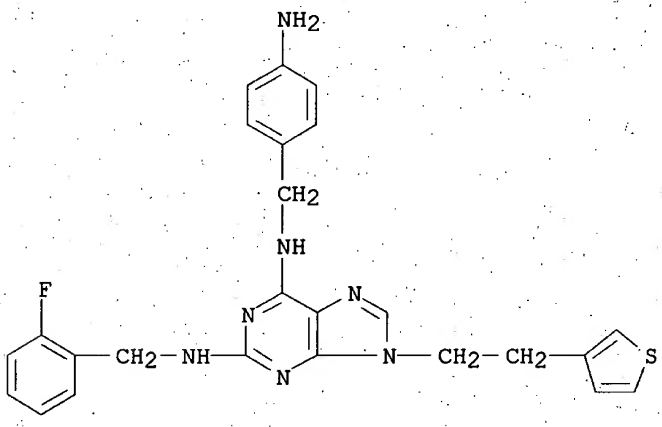
RN 188644-46-4 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(4-aminophenyl)methyl]-N2-(3-aminopropyl)-9-[2-(3-thienyl)ethyl]- (9CI) (CA INDEX NAME)



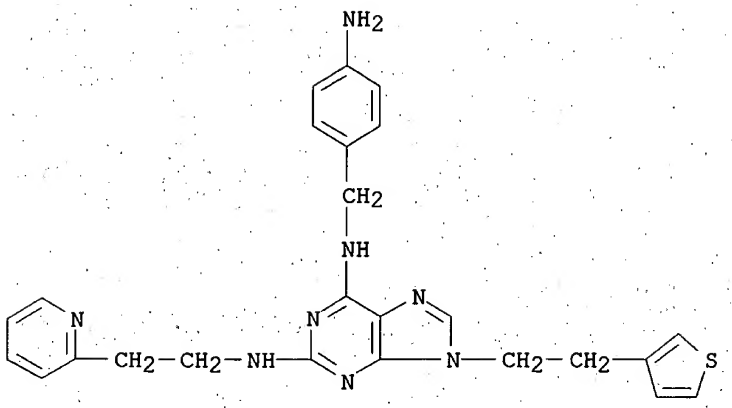
RN 188644-47-5 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(4-aminophenyl)methyl]-N2-[(4-methoxyphenyl)methyl]-9-[2-(3-thienyl)ethyl]- (9CI) (CA INDEX NAME)



RN 188644-48-6 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(4-aminophenyl)methyl]-N2-[(2-fluorophenyl)methyl]-9-[2-(3-thienyl)ethyl]- (9CI) (CA INDEX NAME)

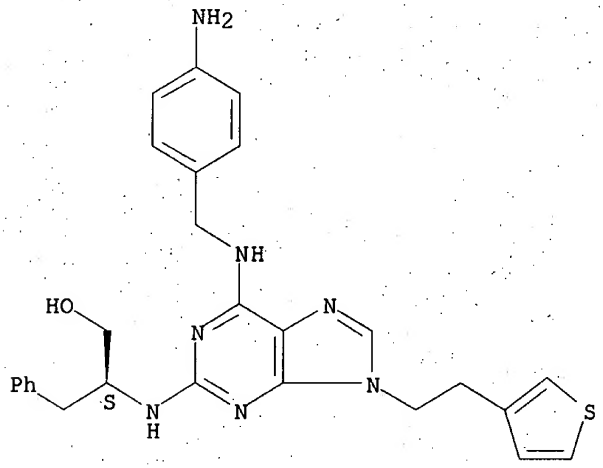


RN 188644-49-7 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(4-aminophenyl)methyl]-N2-[2-(2-pyridinyl)ethyl]-9-[2-(3-thienyl)ethyl]- (9CI) (CA INDEX NAME)

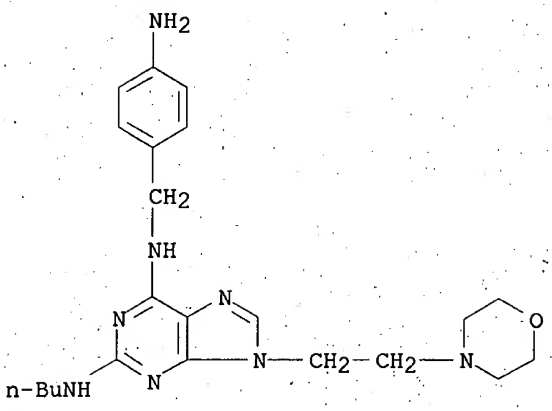


RN 188644-50-0 HCAPLUS
CN Benzenepropanol, .beta.-[[6-[[(4-aminophenyl)methyl]amino]-9-[2-(3-thienyl)ethyl]-9H-purin-2-yl]amino]-, (S)- (9CI) (CA INDEX NAME)

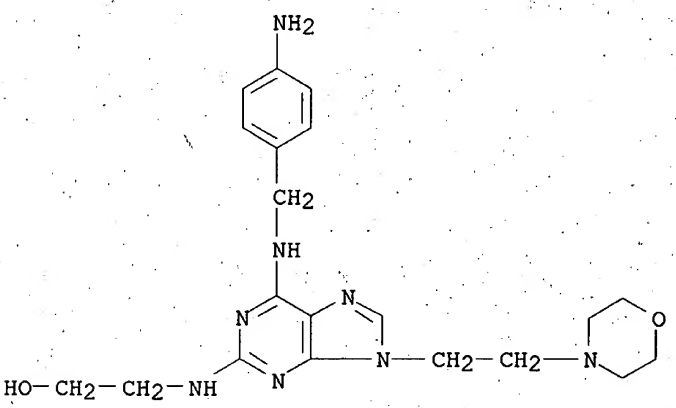
Absolute stereochemistry.



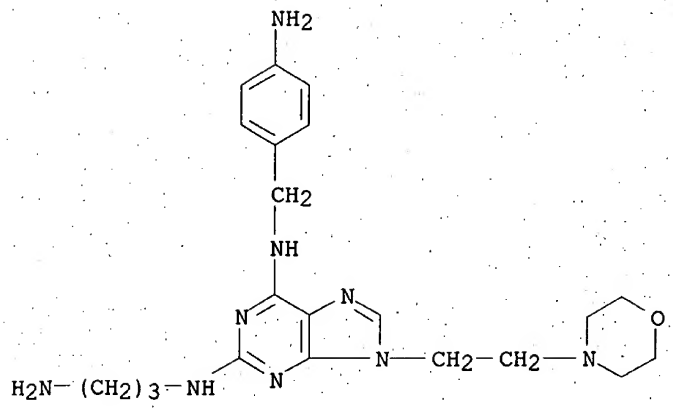
RN 188644-62-4 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(4-aminophenyl)methyl]-N2-butyl-9-[2-(4-morpholinyl)ethyl]- (9CI) (CA INDEX NAME)



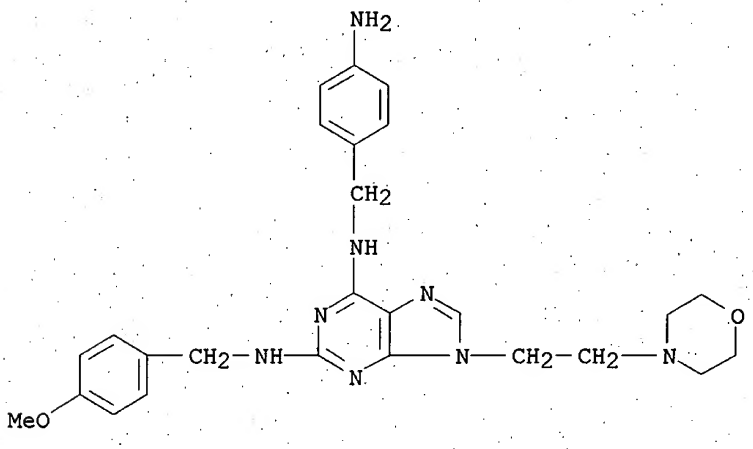
RN 188644-63-5 HCAPLUS
CN Ethanol, 2-[[6-[[(4-aminophenyl)methyl]amino]-9-[2-(4-morpholinyl)ethyl]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



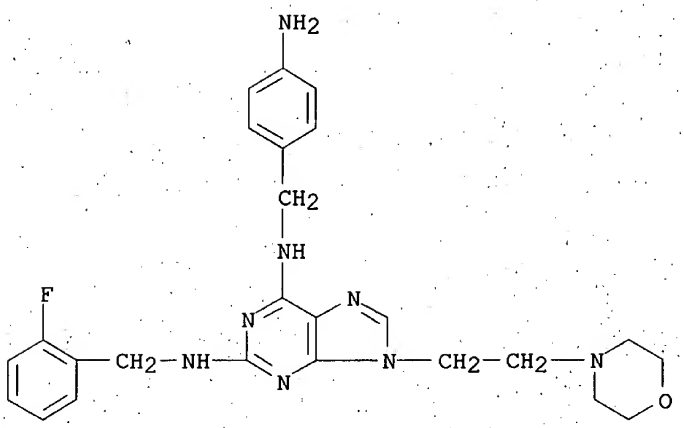
RN 188644-64-6 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(4-aminophenyl)methyl]-N2-(3-aminopropyl)-9-[2-(4-morpholinyl)ethyl]- (9CI) (CA INDEX NAME)



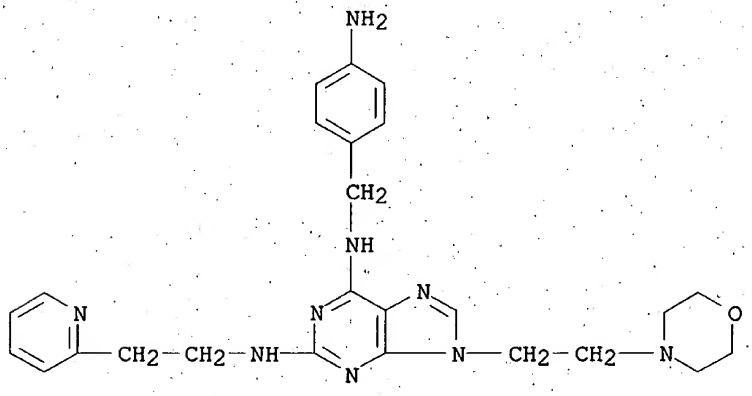
RN 188644-65-7 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(4-aminophenyl)methyl]-N2-[(4-methoxyphenyl)methyl]-9-[2-(4-morpholinyl)ethyl]- (9CI) (CA INDEX NAME)



RN 188644-66-8 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(4-aminophenyl)methyl]-N2-[(2-fluorophenyl)methyl]-9-[2-(4-morpholinyl)ethyl]- (9CI) (CA INDEX NAME)

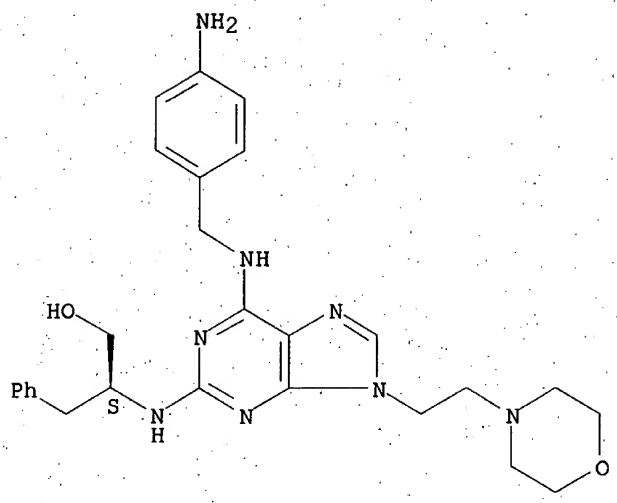


RN 188644-67-9 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(4-aminophenyl)methyl]-9-[2-(4-morpholinyl)ethyl]-N2-[2-(2-pyridinyl)ethyl]- (9CI) (CA INDEX NAME)

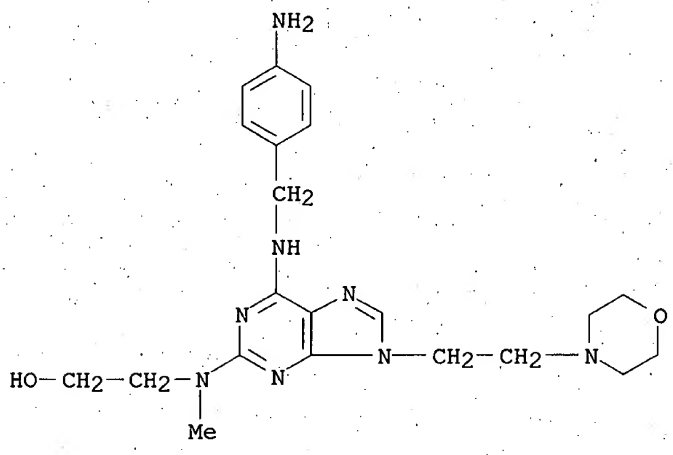


RN 188644-68-0 HCAPLUS
CN Benzenepropanol, .beta.-[[6-[[(4-aminophenyl)methyl]amino]-9-[2-(4-morpholinyl)ethyl]-9H-purin-2-yl]amino]-, (S)- (9CI) (CA INDEX NAME)

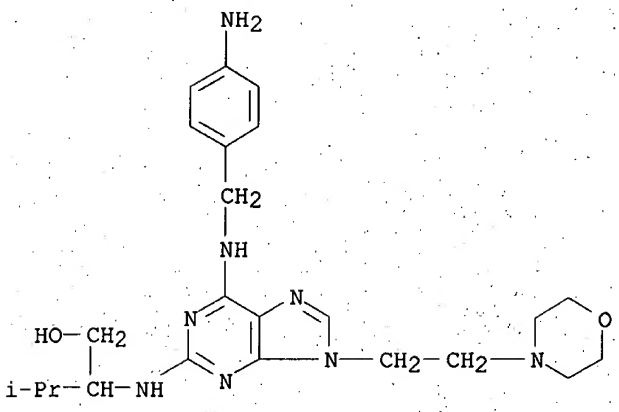
Absolute stereochemistry.



RN 188644-70-4 HCAPLUS
CN Ethanol, 2-[[6-[[(4-aminophenyl)methyl]amino]-9-[2-(4-morpholinyl)ethyl]-9H-purin-2-yl]methylamino]- (9CI) (CA INDEX NAME)

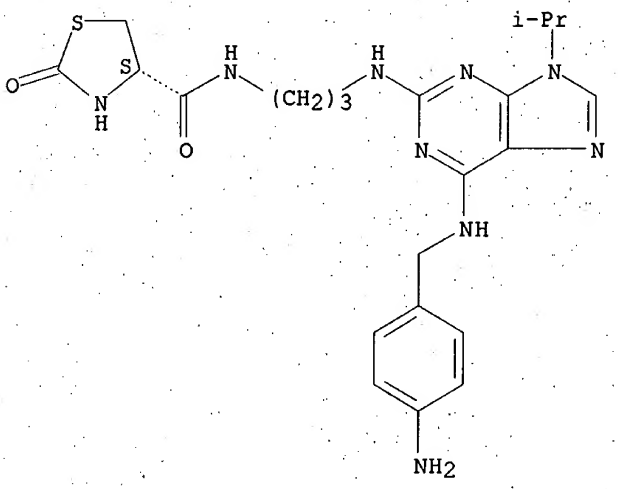


RN 188644-71-5 HCAPLUS
CN 1-Butanol, 2-[[6-[[(4-aminophenyl)methyl]amino]-9-[2-(4-morpholinyl)ethyl]-9H-purin-2-yl]amino]-3-methyl- (9CI) (CA INDEX NAME)

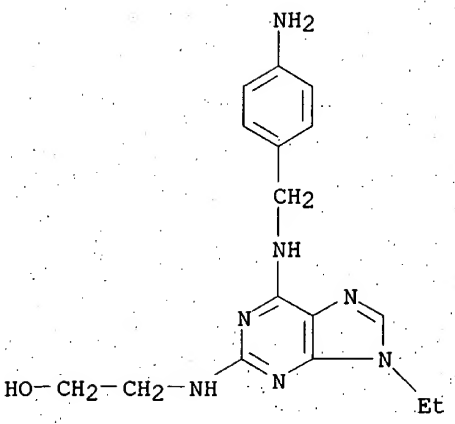


RN 188644-72-6 HCAPLUS
CN 4-Thiazolidinecarboxamide, N-[3-[[6-[[(4-aminophenyl)methyl]amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]propyl]-2-oxo-, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 188644-73-7 HCAPLUS
CN Ethanol, 2-[[6-[[(4-aminophenyl)methyl]amino]-9-ethyl-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



L5 ANSWER 15 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:140835 HCAPLUS
DOCUMENT NUMBER: 126:139488
TITLE: Cytokinin-Derived Cyclin-Dependent Kinase Inhibitors: Synthesis and cdc2 Inhibitory Activity of Olomoucine and Related Compounds
AUTHOR(S): Havlicek, Libor; Hanus, Jan; Vesely, Jaroslav; Leclerc, Sophie; Meijer, Laurent; Shaw, Gordon; Strnad, Miroslav
CORPORATE SOURCE: Central Radioisotope Laboratory Medical Faculty 1, Charles University, Prague, 121 08, Czech Rep.
SOURCE: Journal of Medicinal Chemistry (1997), 40(4), 408-412
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Cyclin-dependent kinases (cdk) have recently raised considerable interest in view of their essential role in the regulation of the cell division cycle. The structure-activity relationships of cdk inhibition showed that the 1, 3, and 7 positions of the purine ring must remain free, probably for a direct interaction, in which it behaves as a hydrogen bond acceptor. Olomoucine (6-(benzylamino)-2-[(2-hydroxyethyl)amino]-9-methylpurine, OC), roscovitine (6-(benzylamino)-2(R)-[[1-(hydroxymethyl)propyl]amino]-9-isopropylpurine), and other N6,2,9-trisubstituted adenines were found to exert a strong inhibitory effect on the p34cdc2/cyclin B kinase. Removal or change of the side chain at position 2 or the hydrophobic group at position 9 dramatically decreased the inhibitory activity of olomoucine or roscovitine. Inhibition of cdk with OC and related compds. clearly arrests cell proliferation of many tumor cell lines at G1/S and G2/M transitions and also triggers apoptosis in the target tumor cells in vitro and in vivo. Thus, from a pharmacol. point of view, OC may represent a model compd. for a new class of antimitotic and antitumor drugs.

CC 1-3 (Pharmacology)
Section cross-reference(s): 28

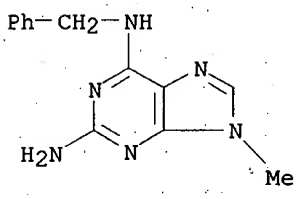
IT 5440-16-4P 77868-58-7P 89897-64-3P **158982-11-7P**
158982-13-9P **158982-15-1P** **158982-16-2P** 186692-38-6P
186692-39-7P **186692-40-0P** 186692-41-1P 186692-42-2P
186692-43-3P **186692-44-4P** **186692-45-5P**
186692-46-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and cdc2 inhibitory activity of olomoucine and related compds.)

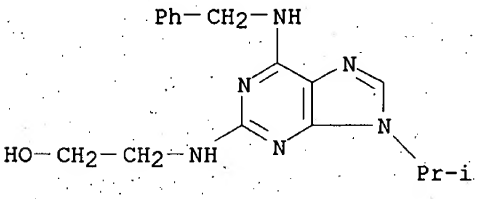
IT 73-24-5, Adenine, biological studies 700-00-5 935-69-3, 6-Amino-7-methylpurine 1214-39-7 1445-08-5 1904-98-9, 1H-Purine-2,6-diamine 5142-22-3 5142-23-4, 6-Amino-3-methylpurine 14671-22-8 14671-24-0 70608-06-9 **101622-51-9**, Olomoucine 101622-53-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(synthesis and cdc2 inhibitory activity of olomoucine and related compds.)

IT **158982-11-7P 158982-15-1P 158982-16-2P 186692-40-0P 186692-43-3P 186692-44-4P 186692-45-5P 186692-46-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(synthesis and cdc2 inhibitory activity of olomoucine and related compds.)

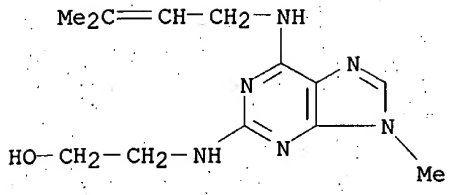
RN 158982-11-7 HCAPLUS
CN 9H-Purine-2,6-diamine, 9-methyl-N6-(phenylmethyl)- (9CI) (CA INDEX NAME)



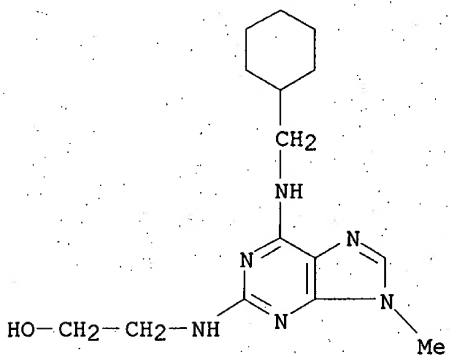
RN 158982-15-1 HCAPLUS
CN Ethanol, 2-[[9-(1-methylethyl)-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



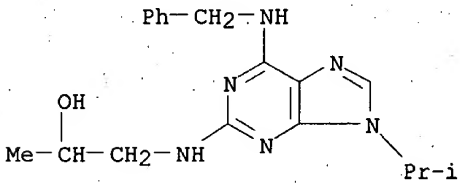
RN 158982-16-2 HCAPLUS
CN Ethanol, 2-[[9-methyl-6-[(3-methyl-2-butenyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



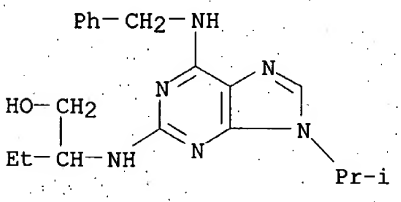
RN 186692-40-0 HCAPLUS
CN Ethanol, 2-[[6-[(cyclohexylmethyl)amino]-9-methyl-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



RN 186692-43-3 HCAPLUS
CN 2-Propanol, 1-[[9-(1-methylethyl)-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)

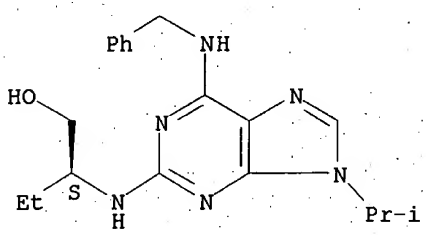


RN 186692-44-4 HCAPLUS
CN 1-Butanol, 2-[[9-(1-methylethyl)-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



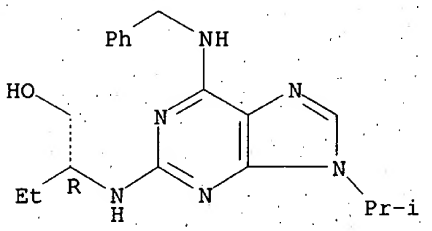
RN 186692-45-5 HCAPLUS
CN 1-Butanol, 2-[[9-(1-methylethyl)-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

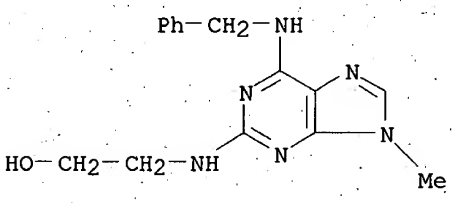


RN 186692-46-6 HCAPLUS
CN 1-Butanol, 2-[[9-(1-methylethyl)-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **101622-51-9**, Olomoucine
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(synthesis and cdc2 inhibitory activity of olomoucine and related compds.)
RN 101622-51-9 HCAPLUS
CN Ethanol, 2-[[9-methyl-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



L5 ANSWER 16 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:26212 HCAPLUS
DOCUMENT NUMBER: 126:74664
TITLE: Facile Preparation of 2,6-Disubstituted Purines Using Solid-Phase Chemistry

AUTHOR(S): Nugiel, David A.; Cornelius, Lyndon A. M.; Corbett, Jeffrey W.
CORPORATE SOURCE: DuPont Merck Pharmaceutical Company, Wilmington, DE, 19880-0500, USA
SOURCE: Journal of Organic Chemistry (1997), 62(1), 201-203
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A solid-phase approach to the prepn. of novel 2,6-disubstituted purines is presented. 2,6-Dichloropurine was loaded onto a THP linked solid support through the N-9 nitrogen. Displacement of the 6-chloro position was accomplished using excess amine at 80.degree. in n-butanol. The 2-chloro position required more forcing conditions and was displaced using an amine as solvent at 150 .degree.C. The final products were cleaved from the resin to give the desired targets in 85-95% crude yield. Various primary and secondary amines, anilines and sulfonamides could be introduced at the 6-position of purine and subsequently modified at the 2-position. This approach was used to prep. olomoucine, a selective p33cdk2/cyclin A inhibitor, in three steps and 60% overall yield.

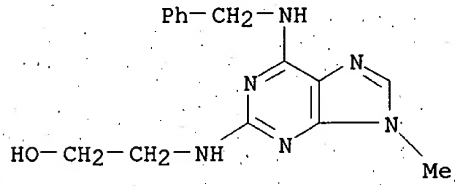
CC 26-9 (Biomolecules and Their Synthetic Analogs)

IT **101622-51-9P**, Olomoucine 185408-98-4P 185409-00-1P 185409-01-2P 185409-02-3P 185409-03-4P 185409-04-5P 185409-05-6P 185409-06-7P 185409-07-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of 2,6-disubstituted purines using solid-phase chem.)

IT **101622-51-9P**, Olomoucine
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of 2,6-disubstituted purines using solid-phase chem.)

RN 101622-51-9 HCAPLUS

CN Ethanol, 2-[[9-methyl-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



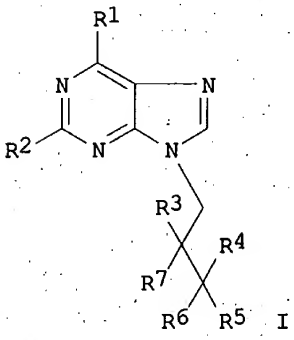
L5 ANSWER 17 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:994374 HCAPLUS
DOCUMENT NUMBER: 124:202289
TITLE: Preparation of purine-substituted hepadnaviridae antiviral agents
INVENTOR(S): Marcuccio, Sebastian Mario; Holan, George; Coghlan, Phillip Albert; Jarvis, Karen Elizabeth; Robertson, Alan Duncan; Turner, Kathleen Anne; Weigold, Helmut
PATENT ASSIGNEE(S): Commonwealth Scientific and Industrial Research Organisation, Australia
SOURCE: PCT Int. Appl., 183 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9522330	A1	19950824	WO 1995-AU76	19950217
W:	AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, UG			
RW:	KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
AU 9518010	A1	19950904	AU 1995-18010	19950217
ZA 9501336	A	19960119	ZA 1995-1336	19950217

PRIORITY APPLN. INFO.: AU 1994-3934 19940217
AU 1994-320 19941223
WO 1995-AU76 19950217

OTHER SOURCE(S): MARPAT 124:202289
GI



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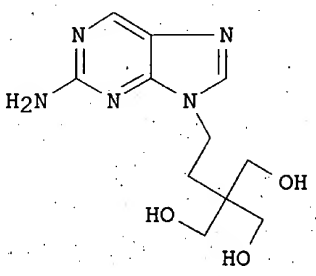

II

AB The title compds. [I; R1 = hydrogen, halogen, hydroxy, azide, (un)substituted alkyl, (un)substituted aryloxy, mercapto, etc.; R2 = hydrogen, hydroxy, azide, (un)substituted alkoxy, (un)substituted aryloxy, mercapto, (un)substituted amino, etc.; R3, R7 = hydrogen, (un)substituted alkyl, halogen, hydroxy, azide, (un)substituted alkoxy, (un)substituted aryloxy, mercapto, (un)substituted thio, (un)substituted amino; R3R7 = :O, :S, :NOH, etc.; R5, R6 = (un)substituted alkyl, halogen, hydroxy, azide, (un)substituted alkoxy, (un)substituted aryloxy, mercapto, etc.; etc.], useful as hepadnaviridae-active antiviral agents, are prepd. and I-contg. formulations presented. Thus, purine deriv. II (m.p. 190-191.degree.) was prepd. from 9-[4-acetoxy-3,3-bis(acetoxymethyl)but-1-yl]-2-aminopurine and demonstrated a EC50 against human hepatitis B virus of 0.16 .mu.M.

IC ICM A61K031-52

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

IT 119117-11-2P 119117-19-0P 119117-33-8P 172644-54-1P 172644-99-4P
172645-00-0P 172645-01-1P 172645-02-2P 172645-03-3P 172645-04-4P
172645-05-5P 172645-06-6P 172645-07-7P 172645-08-8P 172645-09-9P
172645-10-2P 172645-11-3P 172645-12-4P 172645-13-5P 172645-14-6P

172645-15-7P 172645-16-8P 172645-17-9P 172645-18-0P 172645-19-1P
172645-20-4P 172645-21-5P 172645-22-6P 172645-23-7P 172645-24-8P
172645-25-9P 172645-26-0P 172645-27-1P 172645-28-2P 172645-29-3P
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172645-96-4P 172645-97-5P 172645-98-6P 172645-99-7P 172646-00-3P
172646-01-4P 172646-02-5P 172646-03-6P 172646-04-7P 172646-05-8P

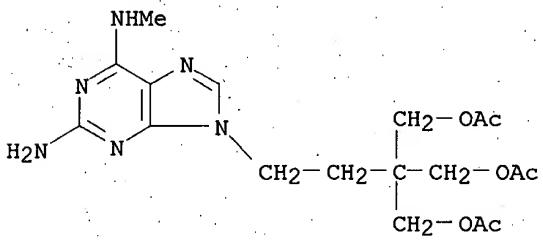
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of purine-substituted hepadnaviridae antiviral agents)

IT **172645-52-2P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of purine-substituted hepadnaviridae antiviral agents)

RN 172645-52-2 HCAPLUS

CN 1,3-Propanediol, 2-[(acetyloxy)methyl]-2-[2-[2-amino-6-(methylamino)-9H-purin-9-yl]ethyl]-, diacetate (ester) (9CI) (CA INDEX NAME)



L5 ANSWER 18 OF 40 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1995:937473 HCAPLUS

DOCUMENT NUMBER: 124:146698

TITLE: Synthesis of enantiomeric N-(2-phosphonomethoxypropyl) derivatives of purine and pyrimidine bases. II. The synthon approach

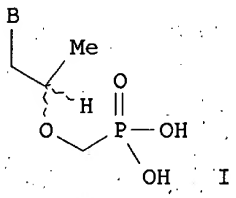
AUTHOR(S): Holy, Antonin; Dvorakova, Hana; Masojidkova, Milena

CORPORATE SOURCE: Institute Organic Chemistry Biochemistry, Academy Sciences Czech Republic, Prague, 166 10, Czech Rep.

SOURCE: Collection of Czechoslovak Chemical Communications (1995), 60(8), 1390-409
CODEN: CCCCAK; ISSN: 0010-0765

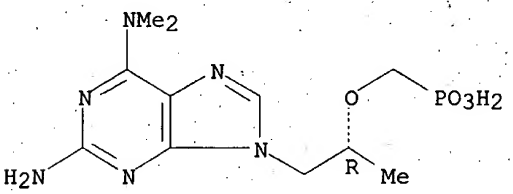
PUBLISHER: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:146698
GI

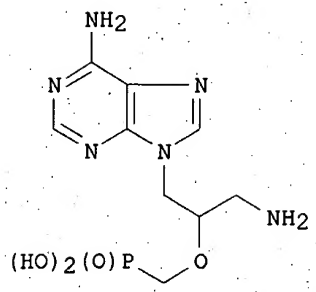


AB Acyclic nucleotides, e.g. I (B = adenine, guanine, hypoxanthine), were prepd. from the corresponding 1-benzyloxy-2-propanol.
CC 33-9 (Carbohydrates)
IT 138247-60-6P 138247-67-3P 147057-09-8P 147057-10-1P 160616-07-9P 160616-08-0P 160616-13-7P 160616-14-8P **160616-15-9P** 173277-55-9P 173277-56-0P 173277-58-2P 173277-59-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of enantiomeric acyclic nucleotide phosphonates)
IT **160616-15-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of enantiomeric acyclic nucleotide phosphonates)
RN 160616-15-9 HCAPLUS
CN Phosphonic acid, [[(1R)-2-[2-amino-6-(dimethylamino)-9H-purin-9-yl]-1-methylethoxy]methyl]- (9CI) (CA INDEX NAME)

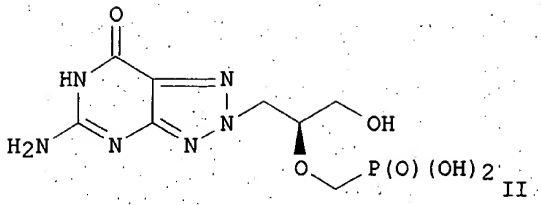
Absolute stereochemistry. Rotation (-).



L5 ANSWER 19 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:631063 HCAPLUS
DOCUMENT NUMBER: 123:286471
TITLE: Acyclic nucleotide analogs and related compounds
AUTHOR(S): Holy, Antonin; Dvorakova, Hana
CORPORATE SOURCE: Inst. of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 166 10, Czech Rep.
SOURCE: Nucleosides & Nucleotides (1995), 14(3-5), 695-702
CODEN: NUNUD5; ISSN: 0732-8311
PUBLISHER: Dekker
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I



II

AB Acyclic nucleotide analogs bearing amino- and N-substituted amino groups in the side chain, e.g. I, were prepd. by alkylation of the bases with corresponding oxiranes and subsequent introduction of phosphonomethyl ether function. Novel enantiomeric synthons for the prepn. of 3-hydroxy-2-phosphonylmethoxypropyl (HPMP)-compds. were prepd. from 1-O-benzyl-(R)-glycerol and applied to syntheses of 8-azaguanine derivs., e.g. II.

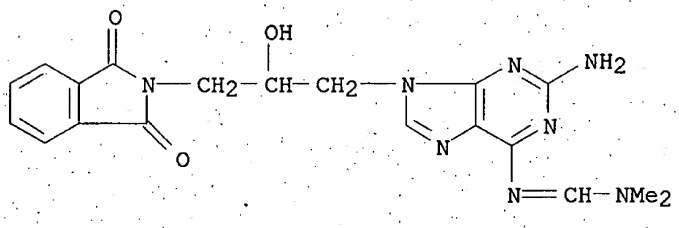
CC 33-9 (Carbohydrates)

IT 151223-09-5P 151223-22-2P 151223-28-8P 169514-89-0P
169514-90-3P 169514-91-4P 169514-92-5P 169514-93-6P
169514-94-7P 169514-96-9P 169514-97-0P 169514-98-1P 169514-99-2P
169515-00-8P 169515-01-9P 169515-02-0P 169515-03-1P 169515-04-2P
169515-05-3P 169515-06-4P 169515-07-5P 169515-14-4P 169515-15-5P
169515-16-6P 169515-17-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of acyclic nucleotide analogs)

IT **169514-90-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of acyclic nucleotide analogs)

RN 169514-90-3 HCAPLUS

CN Methanimidamide, N'-[2-amino-9-[3-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)-2-hydroxypropyl]-9H-purin-6-yl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



L5 ANSWER 20 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:538896 HCAPLUS
DOCUMENT NUMBER: 122:281445
TITLE: Structure-Activity Relationships of 9-Alkyladenine and

Ribose-Modified Adenosine Derivatives at Rat A3 Adenosine Receptors

AUTHOR(S): Jacobson, Kenneth A.; Siddiqi, Suhaib M.; Olah, Mark E.; Ji, Xiao-duo; Melman, Neli; Bellamkonda, Kamala; Meshulam, Yacov; Stiles, Gary L.; Kim, Hea O.

CORPORATE SOURCE: Laboratory of Bioorganic Chemistry, National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD, 20892, USA

SOURCE: Journal of Medicinal Chemistry (1995), 38(10), 1720-35
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

G87

AB 9-Alkyladenine derivs. and ribose-modified N6-benzyladenosine derivs. were synthesized in an effort to identify selective ligands for the rat A3 adenosine receptor and leads for the development of antagonists. The derivs. contained structural features previously detd. to be important for A3 selectivity in adenosine derivs., such as an N6-(3-iodobenzyl) moiety, and were further substituted at the 2-position with halo, amino, or thio groups. Affinity was detd. in radioligand binding assays at rat brain A3 receptors stably expressed in Chinese hamster ovary (CHO) cells, using [125I]AB-MECA (N6-(4-amino-3-iodobenzyl)adenosine-5'-(N-methyluronamide)), and at rat brain A1 and A2a receptors using [3H]-N6-PIA ((R)-N6-phenylisopropyladenosine) and [3H]CGS 21680 (2-[[[4-(2-carboxyethyl)phenyl]ethyl]amino]-5'-(N-ethylcarbamoyl)adenosine), resp. A series of N6-(3-iodobenzyl) 2-amino derivs. indicated that a small 2-alkylamino group, e.g., methylamino, was favored at A3 receptors. N6-(3-Iodobenzyl)-9-methyl-2-(methylthio)adenine was 61-fold more potent than the corresponding 2-Me ether at A3 receptors and of comparable affinity at A1 and A2a receptors, resulting in a 3-6-fold selectivity for A3 receptors. A pair of chiral N6-(3-iodobenzyl) 9-(2,3-dihydroxypropyl) derivs. showed stereoselectivity, with the R-enantiomer favored at A3 receptors by 5.7-fold. 2-Chloro-9-(.beta.-D-erythrofuranosyl)-N6-(3-iodobenzyl)adenine had a Ki value at A3 receptors of 0.28 .mu.M. 2-Chloro-9-[2-amino-2,3-dideoxy-.beta.-D-5-(methylcarbamoyl)arabinofuranosyl]-N6-(3-iodobenzyl)adenine was moderately selective for A1 and A3 vs A2a receptors. A 3'-deoxy analog of a highly A3-selective adenosine deriv. retained selectivity in binding and was a full agonist in the inhibition of adenylyl cyclase mediated via cloned rat A3 receptors expressed in CHO cells. The 3'-OH and 4'-CH2OH groups of adenosine are not required for activation at A3 receptors. A no. of 2',3'-dideoxyadenosines and 9-acyclic-substituted adenines inhibited adenylyl cyclase at the allosteric "P" site.

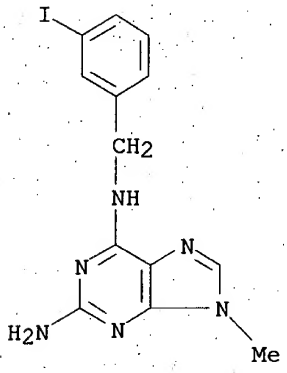
CC 1-3 (Pharmacology)
Section cross-reference(s): 33

IT 58-61-7DP, Adenosine, ribose-modified derivs. 73-24-5DP, Adenine, alkyl derivs. 163042-60-2P 163042-61-3P 163042-62-4P 163042-63-5P 163042-64-6P 163042-65-7P **163042-67-9P** 163042-68-0P **163042-69-1P** **163042-70-4P** **163042-71-5P** **163042-72-6P** 163042-73-7P 163042-74-8P 163042-75-9P 163042-76-0P 163042-78-2P 163042-79-3P 163042-80-6P 163042-81-7P 163042-84-0P 163042-88-4P 163042-89-5P 163042-90-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(structure-activity relationships of alkyladenine and ribose-modified adenosine derivs. at A3 adenosine receptors)

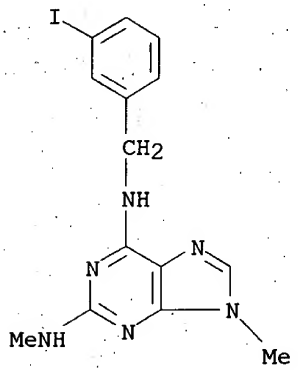
IT **163042-67-9P** **163042-69-1P** **163042-70-4P**

163042-71-5P 163042-72-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(structure-activity relationships of alkyladenine and ribose-modified adenosine derivs. at A3 adenosine receptors)

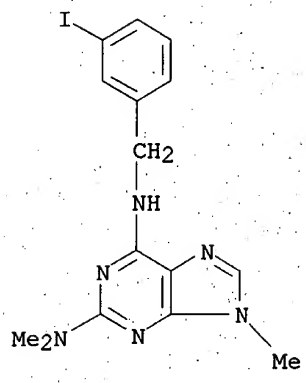
RN 163042-67-9 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(3-iodophenyl)methyl]-9-methyl- (9CI) (CA INDEX NAME)



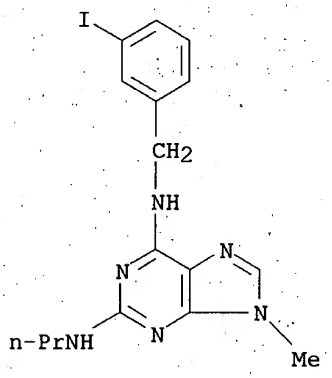
RN 163042-69-1 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(3-iodophenyl)methyl]-N2,9-dimethyl- (9CI) (CA INDEX NAME)



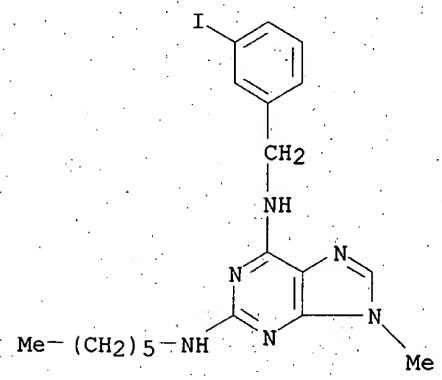
RN 163042-70-4 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(3-iodophenyl)methyl]-N2,N2,9-trimethyl- (9CI) (CA INDEX NAME)



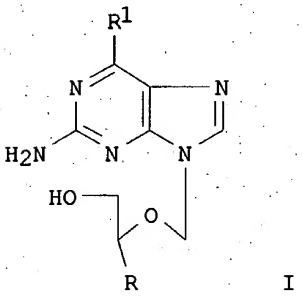
RN 163042-71-5 HCAPLUS
CN 9H-Purine-2,6-diamine, N6-[(3-iodophenyl)methyl]-9-methyl-N2-propyl- (9CI) (CA INDEX NAME)



RN 163042-72-6 HCAPLUS
CN 9H-Purine-2,6-diamine, N2-hexyl-N6-[(3-iodophenyl)methyl]-9-methyl- (9CI) (CA INDEX NAME)



L5 ANSWER 21 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:605863 HCAPLUS
DOCUMENT NUMBER: 121:205863
TITLE: Design and synthesis of 6-fluoropurine acyclonucleosides: potential prodrugs of acyclovir and ganciclovir
AUTHOR(S): Kim, Dae Kee; Kim, Hee Kap; Chae, Young Bok
CORPORATE SOURCE: Korea Res. Inst. Chem. Technol., Daejeon, 305-606, S. Korea
SOURCE: Bioorganic & Medicinal Chemistry Letters (1994), 4(11), 1309-12
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

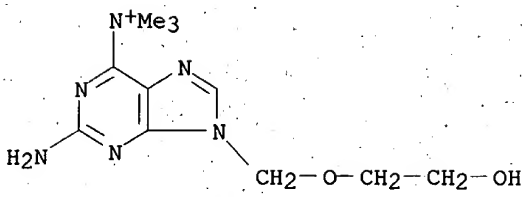
AB 6-Fluoropurine acyclic nucleosides I (R = H, CH2OH, R1 = F) (II) have been prepd. as potential prodrugs of acyclovir and ganciclovir. It has been found that II are 11.6 and 7.6 times more efficiently metabolized to acyclovir and ganciclovir by adenosine deaminase than the corresponding 6-aminopurine acyclonucleosides I (R = H, CH2OH, R1 = NH2).

CC 33-9 (Carbohydrates)
Section cross-reference(s): 7

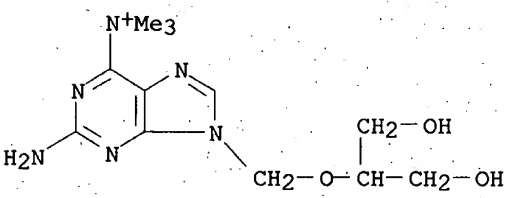
IT **158012-49-8P 158012-50-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, in prepn. of fluoropurine acyclic nucleosides)

IT **158012-49-8P 158012-50-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, in prepn. of fluoropurine acyclic nucleosides)

RN 158012-49-8 HCAPLUS
CN 9H-Purin-6-aminium, 2-amino-9-[(2-hydroxyethoxy)methyl]-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)



RN 158012-50-1 HCAPLUS
CN 9H-Purin-6-aminium, 2-amino-9-[[2-hydroxy-1-(hydroxymethyl)ethoxy]methyl]-N,N,N-trimethyl-, chloride (9CI) (CA INDEX NAME)



L5 ANSWER 22 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1993:496048 HCAPLUS
DOCUMENT NUMBER: 119:96048
TITLE: Syntheses of enantiomeric N-(3-hydroxy-2-phosphonomethoxypropyl) derivatives of purine and pyrimidine bases
AUTHOR(S): Holy, Antonin
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Acad. Sci. Czech Republic, Prague, 166 10, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1993), 58(3), 649-74
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:96048
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Methods of prepn., of N-(3-hydroxy-2-phosphonomethoxypropyl) (HPMP) derivs. of purine and pyrimidine bases with (2S)- and (2R)-configuration, are described. The general method starts from the corresponding

N-(2,3-dihydroxypropyl) derivs. which were converted either into the (R)-enantiomers by reaction of the base with (R)-glycidol butyrate (I) in the presence of cesium carbonate and subsequent methanolysis, or into the (S)-enantiomers by alkylation of the base with (R)-2,2-dimethyl-4-tosyloxymethyl-1,3-dioxolane (II) in the presence of the same reagent. The amino groups on the heterocyclic base in III and IV were benzoylated, via silylation followed by reaction with benzoyl chloride, and the obtained N-benzoates on reaction with trityl chloride afforded the corresponding 3'-O-trityl derivs. These compds. were condensed with bis(2-propyl) p-toluenesulfonyloxymethanephosphonate, 4-MeC6H4SO3CH2P(O)(OCHMe2)2, in DMF in the presence of sodium hydride to give the fully protected diesters. These compds. could be selectively acid-hydrolyzed to remove the trityl group only, or methanolyzed and then acid-hydrolyzed to remove the trityl and N-benzoyl groups, or treated with bromotrimethylsilane to remove the trityl and 2-Pr group to give phosphonates. All the three types of compds. were then converted into free phosphonates of the (S)-series and (R)-series. Derivs. of cytosine, adenine, 2,6-diaminopurine, and guanine were prepd. Condensation of the partially blocked adenine deriv. V (R = Bz, R1 = H) with the tosyl phosphonate deriv. and subsequent deprotection afforded 9-(S)-(2,3-diphosphonomethoxypropyl)adenine [V;R = H, R1 = CH2P(O)(OH)2]. Reaction of the same compd. V (R = Bz, R1 = H) or its (R)-enantiomer with di-Et chlorophosphonate, followed by deblocking, afforded 3'-O-phosphoryl derivs. (S)-HPMPA and (R)-HPMPA. V [R = H, R1 = CH2P(O)(OH)2] showed no antiviral activity.

CC 33-9 (Carbohydrates)

IT 115233-96-0P 148873-47-6P **148873-50-1P** 148967-02-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with diisopropyl (tosyloxymethyl)phosphate)

IT 148873-45-4P, N4-Benzoyl-1-[(R)-2,3-dihydroxypropyl]cytosine **148873-49-8P**, 2,6-Bis(benzoylamino)-9-[(R)-2,3-dihydroxypropyl]purine 148967-04-8P, N2-Benzoyl-9-[(R)-2,3-dihydroxypropyl]guanine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and tritylation of)

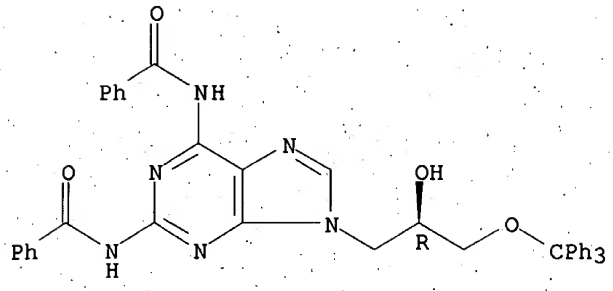
IT 58274-12-7P 127757-35-1P 132336-37-9P **148873-51-2P** 148967-06-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **148873-50-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with diisopropyl (tosyloxymethyl)phosphate)

RN 148873-50-1 HCAPLUS

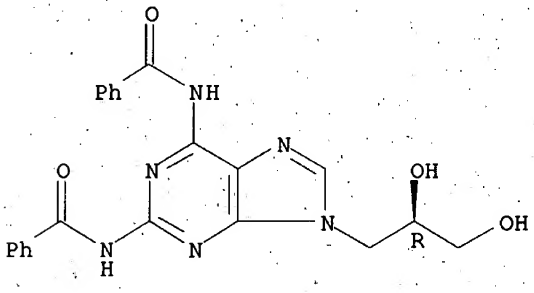
CN Benzamide, N,N'-[9-[2-hydroxy-3-(triphenylmethoxy)propyl]-9H-purine-2,6-diyl]bis-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



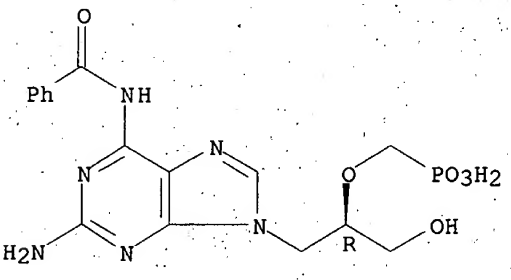
IT **148873-49-8P**, 2,6-Bis(benzoylamino)-9-[(R)-2,3-dihydroxypropyl]purine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and tritylation of)
RN 148873-49-8 HCAPLUS
CN Benzamide, N,N'-[9-(2,3-dihydroxypropyl)-9H-purine-2,6-diyl]bis-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **148873-51-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 148873-51-2 HCAPLUS
CN Phosphonic acid, [[2-[2-amino-6-(benzoylamino)-9H-purin-9-yl]-1-(hydroxymethyl)ethoxy]methyl]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 23 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1991:652157 HCAPLUS
DOCUMENT NUMBER: 115:252157
TITLE: Inhibitors of cytokinin metabolism. Part 4. Substituted xanthines and cytokinin analogs as inhibitors of cytokinin N-glucosylation
AUTHOR(S): Hocart, Charles H.; Letham, David S.; Parker, Charles W.
CORPORATE SOURCE: Res. Sch. Biol. Sci., Aust. Natl. Univ., Canberra, 2601, Australia
SOURCE: Phytochemistry (1991), 30(8), 2477-86
CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of 3-substituted xanthines, 2-(2-hydroxy-2-methylpropylamino)-9-methyl-6-benzylaminopurine and 7-benzylaminooxazolo[5,4-d]pyrimidine were synthesized as potential inhibitors of cytokinin N-glucosylation. In maize leaf segments the latter compd. was the most effective inhibitor tested, inhibiting the formation of the 9-glucoside of 6-benzylaminopurine (BAP) and raising the amt. of free BAP. N-Glucosylation of BAP in radish leaves was suppressed most effectively by 1,7-dimethyl-3-(3-methylbutyl)xanthine, 1,7-dimethyl-3-(5-hexenyl)xanthine and 1,7-dimethyl-3-(3-methyl-2-butenyl)xanthine. The first two compds. were also effective inhibitors in radish cotyledons and elevated the concns. of both free BAP and BAP nucleotide. These results indicate that the structural requirements for effective inhibitors of N-glucosylation differ between the two species.

CC 11-2 (Plant Biochemistry)

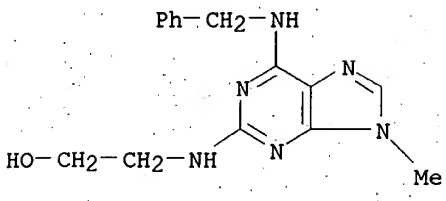
IT 7499-82-3P, 1,7-Dimethyl-3-(3'-methylbutyl)xanthine 7499-88-9P, 1,7,3-Benzylxanthine 69507-18-2P, 1,7-Dimethyl-3-(5'-hexenyl)xanthine 70404-25-0P, 1-Methyl-7-benzylxanthine **101622-51-9P**, 2-(2'-Hydroxyethylamino)-9-methyl-6-benzylaminopurine 121612-37-1P, 1,7-Dimethyl-3-(3'-methyl-2'-butenyl)xanthine 123787-82-6P, 7-Benzylaminooxazolo[5,4-d]pyrimidine 124165-75-9P 124165-76-0P, 1-Methyl-7-(3'-methyl-2'-butenyl)xanthine 124165-77-1P, 1,7-Dimethyl-3-(4'-hydroxybutyl)xanthine 124199-62-8P, 1,7-Dimethyl-3-(3'-methyl-2',3'-dihydroxybutyl)xanthine **137201-13-9P** 137201-19-5P, 1,7-Dimethyl-3-(3'-butenyl)xanthine 137201-20-8P, 1,7-Dimethyl-3-(2'-methyl-2'-propenyl)xanthine 137201-21-9P, (E)-1,7-Dimethyl-3-(4'-hydroxy-3'-methyl-2-butenyl)xanthine 137251-98-0P, 1,7-Dimethyl-3-(4'-pentenyl)xanthine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and glycosylation of cytokinins inhibition by)

IT 101622-53-1P, 2-Chloro-9-methyl-6-benzylaminopurine 137201-22-0P, 2-Chloro-9-methyl-6-benzylmethylaminopurine **137201-23-1P**, 2-Aminomethyl-9-methyl-6-benzylaminopurine
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **101622-51-9P**, 2-(2'-Hydroxyethylamino)-9-methyl-6-benzylaminopurine **137201-13-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and glycosylation of cytokinins inhibition by)

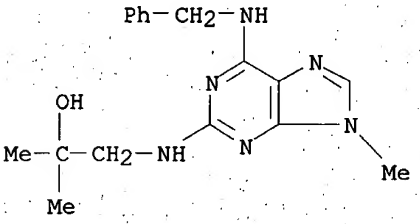
RN 101622-51-9 HCAPLUS
CN Ethanol, 2-[[9-methyl-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI)

(CA INDEX NAME)

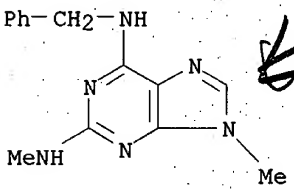


proviso

RN 137201-13-9 HCAPLUS
CN 2-Propanol, 2-methyl-1-[[9-methyl-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



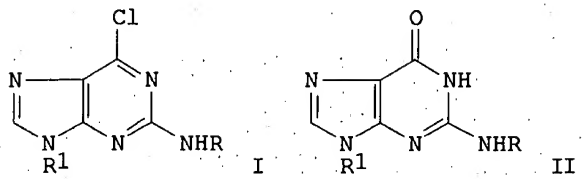
IT **137201-23-1P**, 2-Aminomethyl-9-methyl-6-benzylaminopurine
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 137201-23-1 HCAPLUS
CN 9H-Purine-2,6-diamine, N2,9-dimethyl-N6-(phenylmethyl)- (9CI) (CA INDEX NAME)

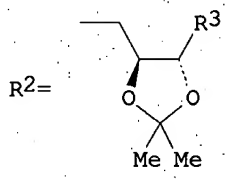


avoids proviso

L5 ANSWER 24 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1990:631075 HCAPLUS
DOCUMENT NUMBER: 113:231075
TITLE: An improved route to guanines substituted at N-9
AUTHOR(S): Ashwell, Mark; Bleasdale, Christine; Golding, Bernard T.; O'Neill, Ian K.
CORPORATE SOURCE: Dep. Chem., Univ,. Newcastle upon Tyne, Newcastle upon Tyne, NE1 7RU, UK
SOURCE: Journal of the Chemical Society, Chemical Communications (1990), (14), 955-6
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English

OTHER SOURCE(S): CASREACT 113:231075
GI





AB 2-Amino-6-chloropurines I [R = H, R1 = Et, CH2CH2OSiMe2CMe2CHMe2; R = (4-MeOC6H4)2CPh, R1 = R2, R3 = CO2Me, CH2OSiPh2CMe3].

CC 26-9 (Biomolecules and Their Synthetic Analogs)

IT 879-08-3P 130584-31-5P 130584-32-6P 130584-33-7P
130584-34-8P 130584-35-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

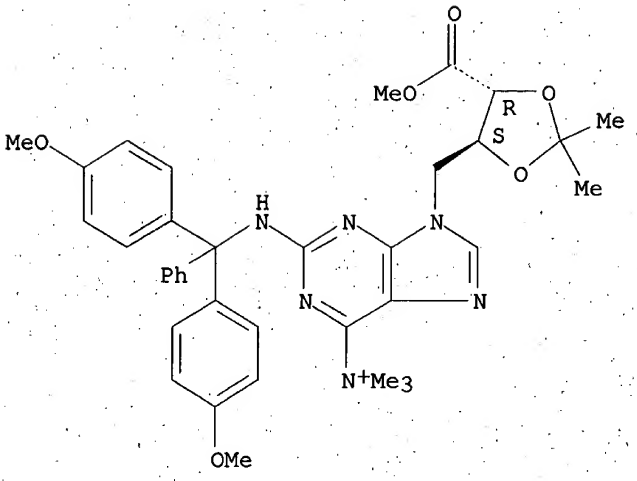
IT **130584-34-8P 130584-35-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 130584-34-8 HCAPLUS

CN 9H-Purin-6-aminium, 2-[[bis(4-methoxyphenyl)phenylmethyl]amino]-9-[[5-(methoxycarbonyl)-2,2-dimethyl-1,3-dioxolan-4-yl]methyl]-N,N,N-trimethyl-, chloride, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A

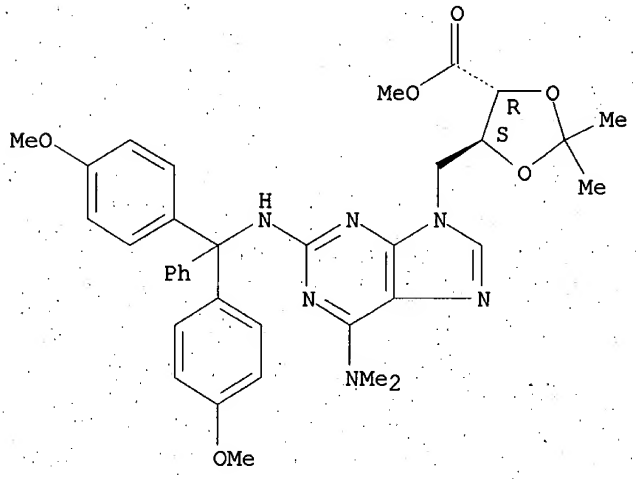


PAGE 2-A

● Cl^-

RN 130584-35-9 HCAPLUS
CN 1,3-Dioxolane-4-carboxylic acid, 5-[[2-[[bis(4-methoxyphenyl)phenylmethyl]amino]-6-(dimethylamino)-9H-purin-9-yl]methyl]-2,2-dimethyl-, methyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

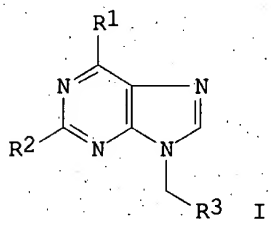


L5 ANSWER 25 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1990:552154 HCAPLUS

DOCUMENT NUMBER: 113:152154
TITLE: Preparation of 9-(halobenzyl)purines as anticonvulsants
INVENTOR(S): Allgeier, Hans
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Eur. Pat. Appl., 33 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 363320	A2	19900411	EP 1989-810731	19890926
EP 363320	A3	19911121		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
IL 91818	A1	19940826	IL 1989-91818	19890928
CA 2000154	AA	19900406	CA 1989-2000154	19891004
FI 8904707	A	19900407	FI 1989-4707	19891004
DD 297820	A5	19920123	DD 1989-333303	19891004
DK 8904913	A	19900407	DK 1989-4913	19891005
NO 8903965	A	19900409	NO 1989-3965	19891005
NO 172986	B	19930628		
NO 172986	C	19931006		
AU 8942612	A1	19900412	AU 1989-42612	19891005
AU 632763	B2	19930114		
ZA 8907587	A	19900530	ZA 1989-7587	19891005
JP 02157279	A2	19900618	JP 1989-258944	19891005
HU 52502	A2	19900728	HU 1989-5224	19891005
US 5110818	A	19920505	US 1990-630401	19901219

PRIORITY APPLN. INFO.: CH 1988-3731 19881006
US 1989-416086 19891002
OTHER SOURCE(S): MARPAT 113:152154
GI



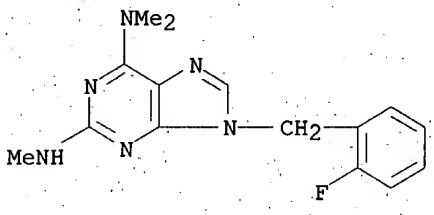
I

AB The title compds. (I; R1 = H, amino, acylamino; R2 = halo, alkoxy, alkyl, amino, acylamino; R3 = halophenyl) with numerous provisos, were prepd. as anticonvulsants (no data). Thus, a mixt. of 2-chloro-6-(N,N-dimethylamino)-9H-purine, 2-fluorobenzyl bromide, and K2CO3 was stirred 3 h in DMF at room temp. to give 2-chloro-6-(N,N-dimethylamino)-9-(2-fluorobenzyl)-9H-purine.
IC ICM C07D473-00
ICS A61K031-52
CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1

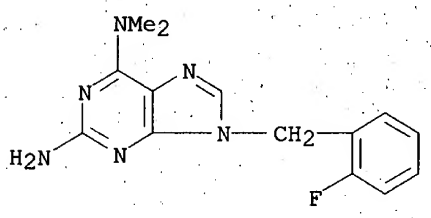
IT 129499-28-1P **129499-29-2P 129499-30-5P**
129499-31-6P 129499-32-7P 129499-33-8P 129499-34-9P
129499-35-0P 129499-36-1P **129499-37-2P 129499-38-3P**
129499-39-4P 129499-40-7P 129499-41-8P **129499-42-9P**
129499-43-0P 129499-44-1P 129499-45-2P 129499-46-3P
129499-47-4P 129499-48-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as anticonvulsant)

IT **129499-29-2P 129499-30-5P 129499-31-6P**
129499-32-7P 129499-37-2P 129499-38-3P
129499-39-4P 129499-42-9P 129499-43-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as anticonvulsant)

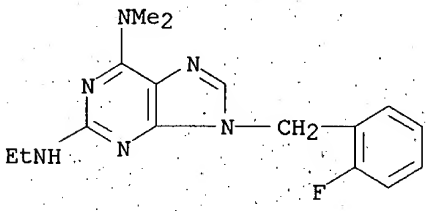
RN 129499-29-2 HCAPLUS
CN 9H-Purine-2,6-diamine, 9-[(2-fluorophenyl)methyl]-N2,N6,N6-trimethyl- (9CI) (CA INDEX NAME)



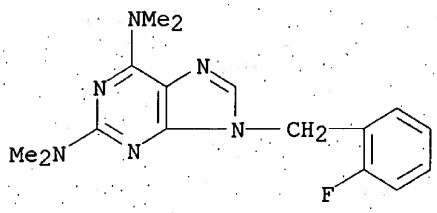
RN 129499-30-5 HCAPLUS
CN 9H-Purine-2,6-diamine, 9-[(2-fluorophenyl)methyl]-N6,N6-dimethyl- (9CI) (CA INDEX NAME)



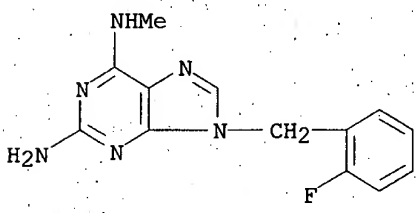
RN 129499-31-6 HCAPLUS
CN 9H-Purine-2,6-diamine, N2-ethyl-9-[(2-fluorophenyl)methyl]-N6,N6-dimethyl- (9CI) (CA INDEX NAME)



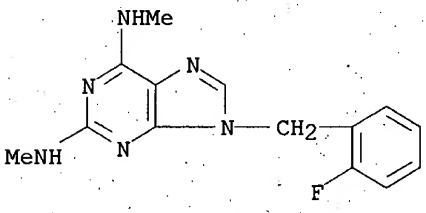
RN 129499-32-7 HCAPLUS
CN 9H-Purine-2,6-diamine, 9-[(2-fluorophenyl)methyl]-N,N,N',N'-tetramethyl- (9CI) (CA INDEX NAME)



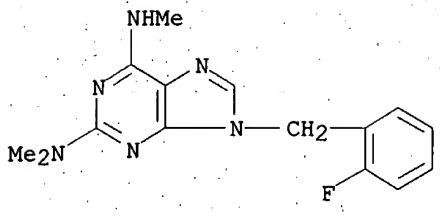
RN 129499-37-2 HCAPLUS
CN 9H-Purine-2,6-diamine, 9-[(2-fluorophenyl)methyl]-N6-methyl- (9CI) (CA INDEX NAME)



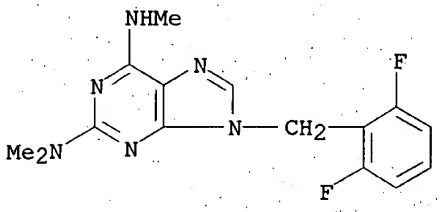
RN 129499-38-3 HCAPLUS
CN 9H-Purine-2,6-diamine, 9-[(2-fluorophenyl)methyl]-N,N'-dimethyl- (9CI) (CA INDEX NAME)



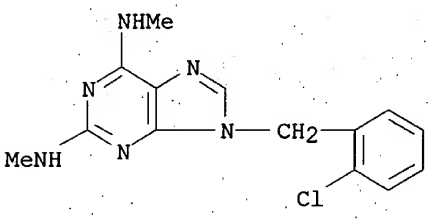
RN 129499-39-4 HCAPLUS
CN 9H-Purine-2,6-diamine, 9-[(2-fluorophenyl)methyl]-N2,N2,N6-trimethyl- (9CI) (CA INDEX NAME)



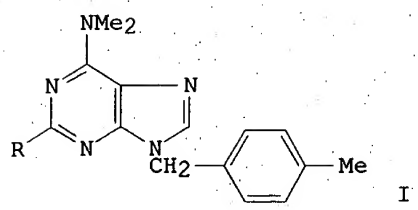
RN 129499-42-9 HCAPLUS
CN 9H-Purine-2,6-diamine, 9-[(2,6-difluorophenyl)methyl]-N2,N2,N6-trimethyl- (9CI) (CA INDEX NAME)



RN 129499-43-0 HCAPLUS
CN 9H-Purine-2,6-diamine, 9-[(2-chlorophenyl)methyl]-N,N'-dimethyl- (9CI) (CA INDEX NAME)



L5 ANSWER 26 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1989:38810 HCAPLUS
DOCUMENT NUMBER: 110:38810
TITLE: Synthesis and structure-activity relationships of 2-substituted-6-(dimethylamino)-9-(4-methylbenzyl)-9H-purines with antirhinovirus activity
AUTHOR(S): Kelley, James L.; Linn, James A.; Selway, J. W. T.
CORPORATE SOURCE: Div. Org. Chem., Burroughs Wellcome Co., Research Triangle Park, NC, 27709, USA
SOURCE: Journal of Medicinal Chemistry (1989), 32(1), 218-24
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:38810
GI



I

AB Purines I (R = F, CF3, Me, Et, NH2, NHMe, NMe2, SMe, SO2Me) were synthesized and tested for antirhinovirus activity to evaluate the effect of 2-substituents on antiviral activity. Intuitive and quant. structure-activity relationship (QSAR) anal. showed that optimum antirhinovirus serotype 1B activity was assocd. with I where R was a lipophilic, electron-withdrawing substituent. The most active compd., I (R = CF3) had an ED50 of 0.03 .mu.M against serotype 1B, but its activity against 18 other serotypes was not uniform; the ED50s ranged over 260-fold.

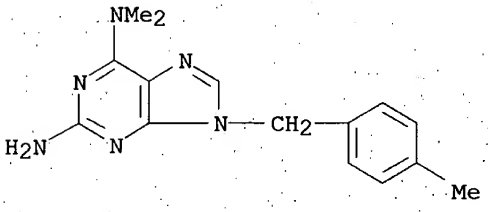
CC 26-9 (Biomolecules and Their Synthetic Analogs)

IT 117860-34-1P 117860-35-2P 117860-36-3P 117860-37-4P
117860-39-6P 117860-40-9P 117860-41-0P
117860-45-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and virucidal activity of)

IT **117860-39-6P 117860-40-9P 117860-41-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and virucidal activity of)

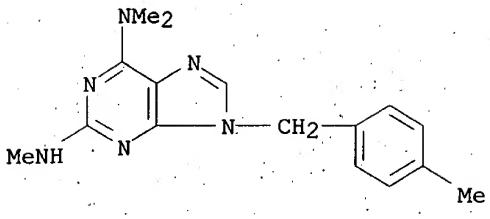
RN 117860-39-6 HCAPLUS

CN 9H-Purine-2,6-diamine, N6,N6-dimethyl-9-[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)

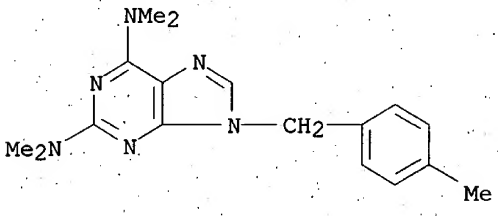


RN 117860-40-9 HCAPLUS

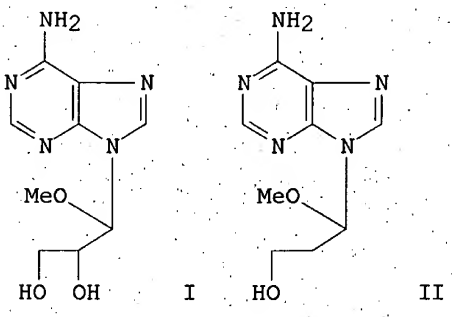
CN 9H-Purine-2,6-diamine, N2,N6,N6-trimethyl-9-[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 117860-41-0 HCAPLUS
CN 9H-Purine-2,6-diamine, N,N,N',N'-tetramethyl-9-[(4-methylphenyl)methyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 27 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1988:438146 HCAPLUS
DOCUMENT NUMBER: 109:38146
TITLE: Novel acyclonucleosides. Part 2. 2,3-Dihydroxy-1-methoxypropyl- and 3-hydroxy-1-methoxypropyl-substituted purines
AUTHOR(S): Bailey, Stuart; Harnden, Michael R.
CORPORATE SOURCE: Biosci. Res. Cent., Beecham Pharm., Great Burgh/Epsom/Surrey, KT18 5XQ, UK
SOURCE: Nucleosides & Nucleotides (1987), 6(3), 555-74
CODEN: NUNUD5; ISSN: 0732-8311
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:38146
GI



I II

AB Several novel purine nucleoside analogs in which the N9-ribosyl moiety is replaced by a 2,3-dihydroxy-1-methoxypropyl or 3-hydroxy-1-methoxypropyl substituent, e.g., I and II, and their N7-isomers were prepd. from the corresponding purines by sequential trimethylsilylation, N-alkylation with AcOCH2CH(OAc)CH(OAc)OMe or AcOCH2CH2CH2CH(OAc)OMe, and deacylation. None of the compds. prepd. showed antiviral activity.

CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 10

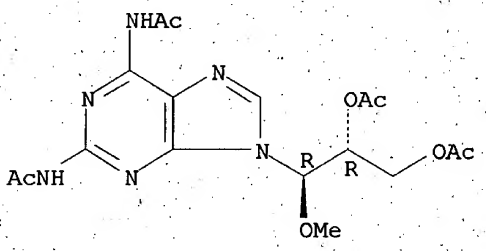
IT 115131-22-1P 115131-23-2P 115131-26-5P 115131-27-6P 115131-29-8P
115131-30-1P **115131-32-3P** 115131-33-4P 115131-35-6P
115131-41-4P 115131-42-5P **115131-45-8P** 115131-46-9P
115131-48-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deacetylation of)

IT **115131-32-3P 115131-45-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deacetylation of)

RN 115131-32-3 HCAPLUS

CN Acetamide, N,N'-[9-[2,3-bis(acetyloxy)-1-methoxypropyl]-9H-purine-2,6-diyl]bis-, (R*,R*)- (9CI) (CA INDEX NAME)

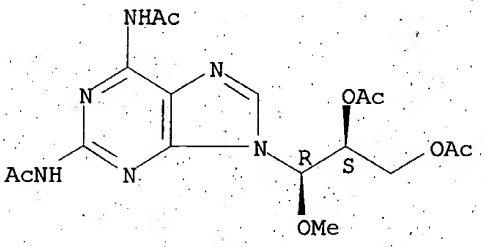
Relative stereochemistry.



RN 115131-45-8 HCAPLUS

CN Acetamide, N,N'-[9-[2,3-bis(acetyloxy)-1-methoxypropyl]-9H-purine-2,6-diyl]bis-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



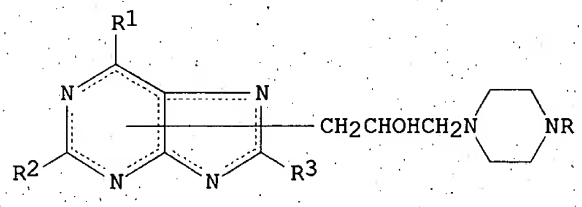
L5 ANSWER 28 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1988:5783 HCAPLUS
DOCUMENT NUMBER: 108:5783
TITLE: Preparation of (diphenylmethylpiperazinyl)alkylpurine

derivatives as cardiotonics and antiarrhythmics
INVENTOR(S): Ott, Hans
PATENT ASSIGNEE(S): Sandoz A.-G., Switz.
SOURCE: Brit. UK Pat. Appl., 11 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2186573	A1	19870819	GB 1987-2937	19870210
GB 2186573	B2	19891122		
NL 8700245	A	19870901	NL 1987-245	19870202
HU 45528	A2	19880728	HU 1987-353	19870202
HU 198052	B	19890728		
FR 2596051	A1	19870925	FR 1987-1670	19870209
FR 2596051	B1	19890526		
CH 668973	A	19890215	CH 1987-460	19870209
US 4849423	A	19890718	US 1987-13516	19870211
FI 8700585	A	19870815	FI 1987-585	19870212
FI 86728	B	19920630		
FI 86728	C	19921012		
DK 8700711	A	19870815	DK 1987-711	19870212
SE 8700555	A	19870815	SE 1987-555	19870212
SE 468643	B	19930222		
AU 8768709	A1	19870820	AU 1987-68709	19870212
AU 590047	B2	19891026		
BE 1000245	A3	19880920	BE 1987-113	19870212
ES 2004218	A6	19881216	ES 1987-353	19870212
AT 8700297	A	19890515	AT 1987-297	19870212
AT 389514	B	19891227		
IL 81546	A1	19900429	IL 1987-81546	19870212
CA 1285559	A1	19910702	CA 1987-529556	19870212
JP 62192381	A2	19870822	JP 1987-32288	19870213
ZA 8701078	A	19880928	ZA 1987-1078	19870213

PRIORITY APPLN. INFO.: DE 1986-3604743 19860214
DE 1986-3612953 19860417

GI



I

AB The title compds. I [R = (un)substituted diphenylalkyl; R1 = H, halo, NH2, (di)alkylamino, 1-piperidino, alkanoylamino, OH, alkoxy, etc.; R2 = H, OH, NH2, alkanoylamino; R3 = H, alkyl, CF3, NH2, halo; dashed line indicates possible double bond positions], useful as cardiotonics and antiarrhythmics, were prepd. by (amino)hydroxypropylation of purine derivs. A mixt. of 13.5 g adenine and 30.8 g 1-diphenylmethyl-4-(2,3-

epoxypropyl)piperazine in 100 mL N caustic soda and 100 mL dioxane was refluxed for 1 h to give (9H)-purine deriv. I (R1 = NH2, R2 = R3 = H, R = Ph2CH, linkage of side chain at position 9 on purine ring), (3H)-purine deriv. I (R, R1-R3 = as given above, linkage of side chain at position 3 on purine ring), and (7H)-purine deriv. I (R, R1-R3 = as given above, linkage of side chain at position 7 on purine ring). At 0.1 mg/kg i.v., (S)-I.2[CH2(CO2H)2] (R1 = MeNH, R2 = R3 = H, R = Ph2CH, linkage at position 9) increased the contractile force of the left ventricle in Inactin-anesthetized rats by 12%, vs. 7% increase by amrinone at the same dose.

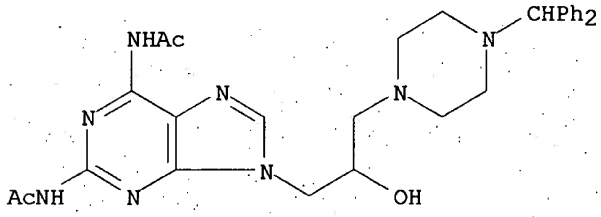
IC ICM C07D473-00
ICS C07D295-08

CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1

IT 111452-37-0P 111452-38-1P 111452-39-2P 111452-40-5P 111452-41-6P
111452-42-7P 111452-43-8P 111452-44-9P 111452-45-0P 111452-46-1P
111452-47-2P 111452-48-3P 111452-49-4P 111452-50-7P 111452-51-8P
111452-52-9P 111452-53-0P 111452-54-1P 111452-56-3P 111452-57-4P
111452-58-5P 111452-59-6P 111452-60-9P 111452-62-1P 111452-64-3P
111452-65-4P 111452-66-5P 111452-68-7P 111452-69-8P 111452-70-1P
111452-71-2P 111487-71-9P 111487-72-0P 111487-73-1P
111487-74-2P 111554-80-4P 111554-81-5P 111554-82-6P 111554-83-7P
111554-84-8P 111554-85-9P 111573-21-8P **111573-22-9P**
111573-23-0P 111573-24-1P 111573-25-2P 111573-26-3P 111573-27-4P
111573-28-5P 111573-29-6P 111573-30-9P 111573-31-0P 111573-32-1P
111573-33-2P 111573-34-3P 111573-35-4P 111573-36-5P 111573-37-6P
111573-38-7P 111573-39-8P 111573-40-1P 111573-41-2P 111573-42-3P
111573-43-4P 111573-44-5P 111573-45-6P 111573-46-7P 111573-47-8P
111573-48-9P 111596-20-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as cardiotonic and antiarrhythmic)

IT **111452-71-2P 111573-22-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as cardiotonic and antiarrhythmic)

RN 111452-71-2 HCAPLUS
CN Acetamide, N,N'-[9-[3-[4-(diphenylmethyl)-1-piperazinyl]-2-hydroxypropyl]-9H-purine-2,6-diyl]bis- (9CI) (CA INDEX NAME)



RN 111573-22-9 HCAPLUS

L5 ANSWER 29 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1987:636373 HCAPLUS
DOCUMENT NUMBER: 107:236373
TITLE: Purine derivatives, their preparation, and their use as cardiotonics and antiarrhythmics
INVENTOR(S): Ott, Hans
PATENT ASSIGNEE(S): Sandoz-Patent-G.m.b.H., Fed. Rep. Ger.

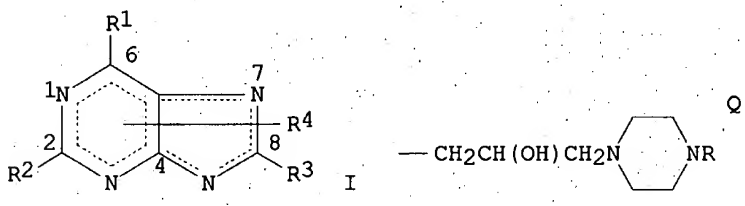
SOURCE: Ger. Offen., 8 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

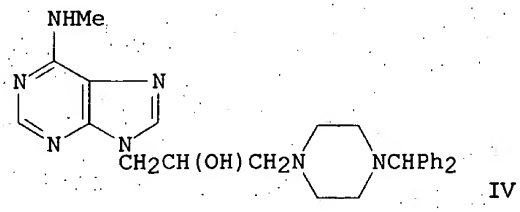
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3703633	A1	19870820	DE 1987-3703633	19870206
NL 8700245	A	19870901	NL 1987-245	19870202
HU 45528	A2	19880728	HU 1987-353	19870202
HU 198052	B	19890728		
FR 2596051	A1	19870925	FR 1987-1670	19870209
FR 2596051	B1	19890526		
CH 668973	A	19890215	CH 1987-460	19870209
US 4849423	A	19890718	US 1987-13516	19870211
FI 8700585	A	19870815	FI 1987-585	19870212
FI 86728	B	19920630		
FI 86728	C	19921012		
DK 8700711	A	19870815	DK 1987-711	19870212
SE 8700555	A	19870815	SE 1987-555	19870212
SE 468643	B	19930222		
AU 8768709	A1	19870820	AU 1987-68709	19870212
AU 590047	B2	19891026		
BE 1000245	A3	19880920	BE 1987-113	19870212
ES 2004218	A6	19881216	ES 1987-353	19870212
AT 8700297	A	19890515	AT 1987-297	19870212
AT 389514	B	19891227		
IL 81546	A1	19900429	IL 1987-81546	19870212
CA 1285559	A1	19910702	CA 1987-529556	19870212
JP 62192381	A2	19870822	JP 1987-32288	19870213
ZA 8701078	A	19880928	ZA 1987-1078	19870213

PRIORITY APPLN. INFO.: DE 1986-3604743 19860214
DE 1986-3612953 19860417

OTHER SOURCE(S): CASREACT 107:236373

GI





AB Purine derivs. I [R1 = H, F, Cl, Br, (di)(alkyl)amino, piperidino, alkanoylamino, SH, OH, alkoxy, alkylthio, BzNH, pyridinylcarbonylamino; R2 = H, OH, (alkanoyl)amino; R3 = H, alkyl, CF3, NH2, F, Cl, Br; R4 = Q; R = (un)substituted diphenylalkyl] and their salts, useful as cardiotonics or antiarrhythmics, were prepd. Adenine was refluxed with 1-(diphenylmethyl)-4-(2,3-epoxypropyl)piperazine (III) in N NaOH and dioxane 1 h to give 3 products which were sepd. by chromatog.: 6-amino-.alpha.-[[4-(diphenylmethyl)-1-piperazinyl]methyl]-9H-purine-9-ethanol, -3H-purine-3-ethanol, and -7H-purine-7-ethanol. The contractile strength of the left heart ventricle of the rat increased 12% at 0.1 or 61% at 1.0 mg IV/kg i.v. The corresponding values for Amrinone were 7% and 29%.

IC ICM C07D473-34
ICS C07D473-30; C07D473-40; C07D303-36; C07D295-08; C07D473-38; A61K031-52

ICA C07D473-00; C07D473-16; C07D473-20; C07D473-24

ICI C07D473-34, C07D213-81

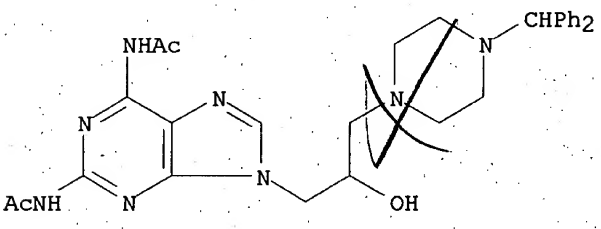
CC 26-9 (Biomolecules and Their Synthetic Analogs)
Section cross-reference(s): 1

IT 111452-37-0P 111452-38-1P 111452-39-2P 111452-40-5P 111452-41-6P
111452-42-7P 111452-43-8P 111452-44-9P 111452-45-0P 111452-46-1P
111452-47-2P 111452-48-3P 111452-49-4P 111452-50-7P 111452-51-8P
111452-52-9P 111452-54-1P 111452-56-3P 111452-57-4P 111452-58-5P
111452-59-6P 111452-61-0P 111452-62-1P 111452-63-2P 111452-64-3P
111452-65-4P 111452-67-6P 111452-68-7P 111452-69-8P 111452-70-1P
111452-71-2P 111487-71-9P 111487-73-1P 111487-74-2P
111554-81-5P 111554-83-7P 111554-84-8P 111554-85-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as cardiotonic or antiarrhythmic)

IT **111452-71-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as cardiotonic or antiarrhythmic)

RN 111452-71-2 HCAPLUS

CN Acetamide, N,N'-[9-[3-[4-(diphenylmethyl)-1-piperazinyl]-2-hydroxypropyl]-9H-purine-2,6-diyl]bis- (9CI) (CA INDEX NAME)



L5 ANSWER 30 OF 40 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1986:164159 HCAPLUS

DOCUMENT NUMBER: 104:164159

TITLE: Inhibition of cytokinin metabolism. Part 1. Inhibitors of two enzymes which metabolize cytokinins

AUTHOR(S): Parker, Charles W.; Entsch, Barrie; Letham, David S.

CORPORATE SOURCE: Res. Sch. Biol. Sci., Aust. Natl. Univ., Canberra, 2601, Australia

SOURCE: Phytochemistry (Elsevier) (1986), 25(2), 303-10

CODEN: PYTCAS; ISSN: 0031-9422
DOCUMENT TYPE: Journal
LANGUAGE: English

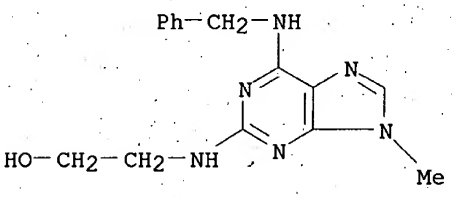
AB Compds. that inhibit the natural metabolic inactivation of cytokinins are of considerable physiol. significance. In this study, inhibitors were found for 2 enzymes that form glucose and alanine conjugates of cytokinin bases, namely, cytokinin 7-glucosyltransferase (I) and .beta.-(9-cytokinin)alanine synthase (II). The most effective inhibitors found for I were the cytokinin analogs 3-methyl-7-n-pentylaminopyrazolo[4,3-d]pyrimidine, which acted competitively (Ki, 22 .mu.M), and the diaminopurine 6-benzylamino-2-(2-hydroxyethylamino)-9-methylpurine (Ki, 3.3 .mu.M). However, these compds. were ineffective as inhibitors of II, which was inhibited competitively by IAA (Ki, 70 .mu.M) and related compds., esp. 5,7-dichloro-IAA (Ki, 0.4 .mu.M). Certain urea derivs. were moderately effective inhibitors of the enzymes (Ki, .apprx.100 .mu.M).

CC 7-3 (Enzymes)
Section cross-reference(s): 11

IT 967-01-1P 101622-50-8P **101622-51-9P** 101622-54-2P
101622-55-3P 101622-56-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and kinetics of cytokinin glucosyltransferase inhibition by)

IT **101622-51-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and kinetics of cytokinin glucosyltransferase inhibition by)

RN 101622-51-9 HCAPLUS
CN Ethanol, 2-[[9-methyl-6-[(phenylmethyl)amino]-9H-purin-2-yl]amino]- (9CI) (CA INDEX NAME)



provided

L5 ANSWER 31 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1985:505266 HCAPLUS
DOCUMENT NUMBER: 103:105266
TITLE: Purine derivatives and their application in anti-viral compositions
INVENTOR(S): Tolman, Richard L.; Ashton, Wallace; Maccoss, Malcolm
PATENT ASSIGNEE(S): Merck and Co., Inc. , USA
SOURCE: Eur. Pat. Appl., 35 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

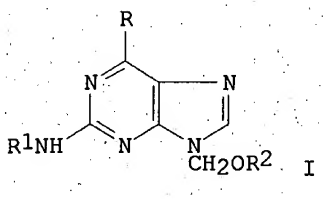
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 138683	A2	19850424	EP 1984-401901	19840924
EP 138683	A3	19880120		

R: CH, DE, FR, GB, IT, LI, NL

JP 60092286	A2	19850523	JP 1984-203023	19840929
US 4897479	A	19900130	US 1988-165360	19880229
PRIORITY APPLN. INFO.:			US 1983-538019	19830930
			US 1985-793080	19851031
			US 1987-40698	19870420

OTHER SOURCE(S): CASREACT 103:105266

GI



I

AB Purines I [R = halogen, SH, alkylthio, OMe, PhSO3, alkylbenzenesulfonyloxy, amino; R1 = H, C1-8 alkanoyl, Bz; R2 = CH(CH2OR3)CH2OR4, CH2CH(OR3)CH2OR4; R3,R4 = H, P(O)(OR5)OR6; R5,R6 = cation, H; R5R6 = P(O)OR7; R7 = H, cation] were prepd. Thus, 2-amino-6-chloropurine was acetylated and treated with AcOCH2OCH(CH2OAc)2 to give I [R = Cl, R1 = Ac, R2 = CH(CH2OAc)2] which was aminated with NH3 to give I [R = NH2, R1 = H, R2 = CH(CH2OH)2]. The latter compd. was converted to its cyclic phosphate with POCl3-(EtO)3PO.

IC ICM C07D473-16
ICS C07D473-18; C07D473-24; C07D473-40; C07F009-65; A61K031-52

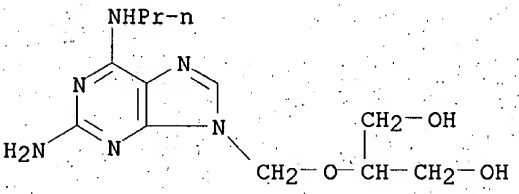
CC 33-9 (Carbohydrates)
Section cross-reference(s): 63

IT 86629-59-6P 88110-70-7P 89419-25-0P 93503-30-1P 93834-95-8P
97965-45-2P 97965-46-3P 97965-47-4P 97965-48-5P **97965-49-6P**
97965-50-9P 97965-51-0P 98936-74-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **97965-49-6P 97965-50-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

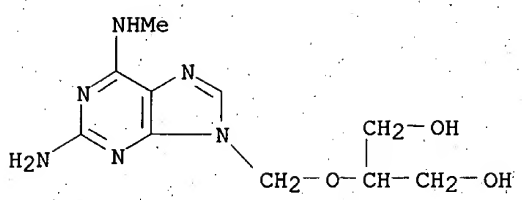
RN 97965-49-6 HCAPLUS

CN 1,3-Propanediol, 2-[[2-amino-6-(propylamino)-9H-purin-9-yl]methoxy]- (9CI) (CA INDEX NAME)

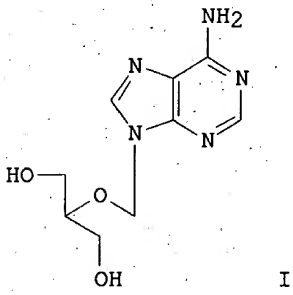


RN 97965-50-9 HCAPLUS

CN 1,3-Propanediol, 2-[[2-amino-6-(methylamino)-9H-purin-9-yl]methoxy]- (9CI) (CA INDEX NAME)



L5 ANSWER 32 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1984:139546 HCAPLUS
DOCUMENT NUMBER: 100:139546
TITLE: Antiviral and ring-open nucleoside analogs. Part V. Synthesis of a purine acyclonucleoside series having pronounced antiviral activity. The glyceropurines
AUTHOR(S): Ogilvie, Kelvin K.; Nghe Nguyen Ba; Gillen, Michael F.; Radatus, Bruno K.; Cheriyan, Ukken O.; Smith, Kendall O.; Galloway, Karen S.
CORPORATE SOURCE: Dep. Chem., McGill Univ., Montreal, QC, H3A 2K6, Can.
SOURCE: Canadian Journal of Chemistry (1984), 62(2), 241-52
CODEN: CJCHAG; ISSN: 0008-4042
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

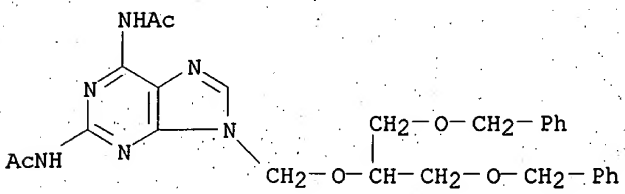
AB A series of purine analogs of the acyclonucleoside I was prepd. Compds. in this series have pronounced activity against herpes virus. These compds. have been designated "glycerosides". Nucleotides were constructed contg. I. These nucleotides are resistant to degrdn. by phosphodiesterases. I is both a poor substrate and a poor inhibitor of adenosine deaminase.

CC 33-9 (Carbohydrates)
Section cross-reference(s): 1

IT **89419-13-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deacetylation of)

IT **89419-13-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(prepn. and deacetylation of)
RN 89419-13-6 HCAPLUS
CN Acetamide, N,N'-[9-[[2-(phenylmethoxy)-1-[(phenylmethoxy)methyl]ethoxy]methyl]-9H-purine-2,6-diyl]bis- (9CI) (CA INDEX NAME)



L5 ANSWER 33 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1983:471134 HCAPLUS
DOCUMENT NUMBER: 99:71134
TITLE: Antiviral compounds
INVENTOR(S): Schaeffer, Howard John
PATENT ASSIGNEE(S): Wellcome Foundation Ltd., UK
SOURCE: Eur. Pat. Appl., 37 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

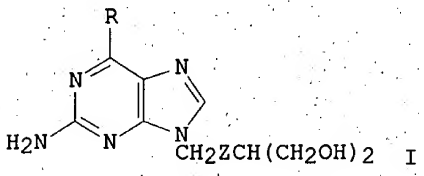
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 72027	A1	19830216	EP 1982-107247	19820810
EP 72027	B1	19880518		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
FI 8202783	A	19830212	FI 1982-2783	19820810
FI 76086	B	19880531		
FI 76086	C	19880909		
DK 8203590	A	19830212	DK 1982-3590	19820810
DK 154561	B	19881128		
DK 154561	C	19890424		
NO 8202725	A	19830214	NO 1982-2725	19820810
NO 158539	B	19880620		
NO 158539	C	19880928		
GB 2104070	A1	19830302	GB 1982-22977	19820810
GB 2104070	B2	19850814		
JP 58041879	A2	19830311	JP 1982-139086	19820810
JP 04000989	B4	19920109		
AU 8287020	A1	19830505	AU 1982-87020	19820810
AU 569462	B2	19880204		
HU 26818	O	19830928	HU 1982-2577	19820810
HU 189609	B	19860728		
DD 202717	A5	19830928	DD 1982-242394	19820810
ES 514877	A1	19831001	ES 1982-514877	19820810
ZA 8205792	A	19840328	ZA 1982-5792	19820810
AT 8203060	A	19850915	AT 1982-3060	19820810
AT 380252	B	19860512		
PL 141198	B1	19870731	PL 1982-237847	19820810

PL 141281	B1	19870731	PL 1982-247393	19820810
AT 34393	E	19880615	AT 1982-107247	19820810
CA 1305138	A1	19920714	CA 1982-409132	19820810
ES 521551	A1	19841216	ES 1983-521551	19830415
ES 521550	A1	19850416	ES 1983-521550	19830415
AT 8401188	A	19850915	AT 1984-1188	19840409
AT 380253	B	19860512		
AT 8401189	A	19850915	AT 1984-1189	19840409
AT 380254	B	19860512		

PRIORITY APPLN. INFO.: GB 1981-24444 19810811
AT 1982-3060 19820810
EP 1982-107247 19820810

OTHER SOURCE(S): CASREACT 99:71134

GI



I

AB Antiviral purines I (R = OH, NH2; Z = O, S) were prepd. Thus, 2,6,9-tris(trimethylsilyl)guanine was refluxed with 1,3-bis(benzyloxy)-2-(chloromethoxy)propane in PhMe in the presence of Et3N to give 9-[[2-benzyloxy-1-(benzyloxymethyl)ethoxy]methyl]guanine, which was debenzylated with Na and liq. NH3 to give I (R = OH, Z = O) (II). In comparison with acyclovir, which generally required a dose rate of 100 mg/kg/day (i.p.) for 5 days to prevent any equine rhinopneumonitis virus-induced mortality, II at 2 mg/kg/day (i.p.) gave complete control.

IC C07D473-16; C07D473-18; A61K031-52

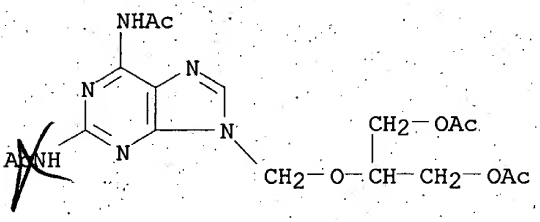
CC 33-9 (Carbohydrates)
Section cross-reference(s): 1, 63

IT 86629-56-3P **86629-64-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deacetylation of)

IT **86629-64-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deacetylation of)

RN 86629-64-3 HCAPLUS

CN Acetamide, N,N'-[9-[[2-(acetyloxy)-1-[(acetyloxy)methyl]ethoxy]methyl]-9H-purine-2,6-diyl]bis- (9CI) (CA INDEX NAME)



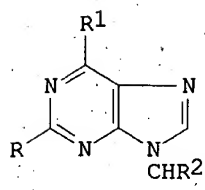
L5 ANSWER 34 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1980:586414 HCAPLUS
DOCUMENT NUMBER: 93:186414
TITLE: Compositions for treating viral infections and guanine acyclic nucleosides
INVENTOR(S): Schaeffer, Howard J.
PATENT ASSIGNEE(S): Burroughs Wellcome Co., USA
SOURCE: U.S., 14 pp. Cont.-in-part of U.S. Ser. No. 608,263, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 8
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4199574	A	19800422	US 1976-662900	19760301
GB 1523865	A	19780906	GB 1974-38278	19740902
US 4146715	A	19790327	US 1977-773135	19770228
CS 203094	P	19810227	CS 1977-3124	19770512
CS 203095	P	19810227	CS 1977-3125	19770512
AT 7706101	A	19790615	AT 1977-6101	19770823
AT 354463	B	19790110		
AT 352751	B	19791010	AT 1977-6103	19770823
AT 7706103	A	19790315		
AT 353804	B	19791210	AT 1977-6104	19770823
AT 7706104	A	19790515		
AT 7706102	A	19791215	AT 1977-6102	19770823
AT 357565	B	19800725		
PL 108512	B1	19800430	PL 1977-200483	19770826
US 4294831	A	19811013	US 1978-874060	19780201
US 4323573	A	19820406	US 1978-874130	19780201
US 4360522	A	19821123	US 1978-874067	19780201
US 4287188	A	19810901	US 1978-920625	19780629
AT 7901040	A	19800915	AT 1979-1040	19790212
AT 361941	B	19810410		

PRIORITY APPLN. INFO.:

GB 1974-38278	19740902
US 1975-608263	19750827
AT 1975-6763	19750902
CS 1975-5957	19750902
US 1976-662900	19760301
US 1976-718105	19760827
US 1977-771778	19770224
US 1977-773135	19770228

GI



$CHR^2ZCHR^3CHR^4R^5$ I

AB Purines I [Z = S, O; R = NH2; R1 = OH; R2 = H, alkyl, hydroxyalkyl; R3 = H, alkyl, hydroxyalkyl, benzyloxyalkyl, Ph; R4 = H, OH, alkyl; R5 = H, OH, NH2, alkyl, hydroxyalkyl, BzO, benzoyloxyalkyl, PhCH2O, OSO2NH2, OP(O)(OH)2, carboxypropionyloxy, AcO] were prepd. by different methods; I (R = R1 = NH2, Z = O, R5 = OH, R2 = R3 = R4 = H), which showed antiviral activity, was among the compds. prepd. 6-Chloropurine was alkylated to give 6-chloro-9-(2-benzoyloxyethoxymethyl)purine, and ammonolysis of the product gave 9-(2-hydroxyethoxymethyl)adenine.

IC A61K031-52; C07D413-18

NCL 424200000

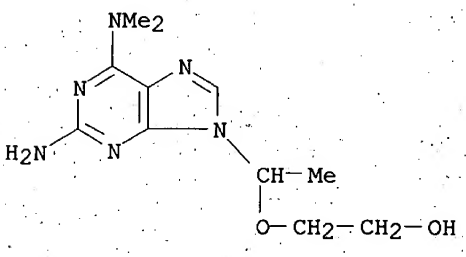
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 31383-66-1P 59277-89-3P 59277-93-9P 59277-95-1P 59277-97-3P
59278-01-2P 59278-02-3P 59278-04-5P 59278-07-8P 59278-08-9P
59278-11-4P 59278-12-5P 59278-13-6P 59298-42-9P 64843-75-0P
64843-76-1P 74554-15-7P 75128-42-6P 75128-44-8P 75128-45-9P
75128-46-0P 75128-47-1P 75128-48-2P 75128-49-3P 75128-50-6P
75128-51-7P 75128-52-8P 75128-53-9P 75128-54-0P 75128-55-1P
75128-56-2P 75128-57-3P 75128-58-4P 75128-59-5P 75128-60-8P
75128-61-9P 75128-62-0P **75128-63-1P** 75128-64-2P
75128-65-3P 75128-66-4P 75128-67-5P 75128-68-6P 75128-69-7P
75128-70-0P 75128-71-1P 75128-72-2P 75128-73-3P 75128-78-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **75128-63-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 75128-63-1 HCAPLUS

CN Ethanol, 2-[1-[2-amino-6-(dimethylamino)-9H-purin-9-yl]ethoxy]- (9CI) (CA INDEX NAME)



L5 ANSWER 35 OF 40 HCAPLUS COPYRIGHT 2003 ACS

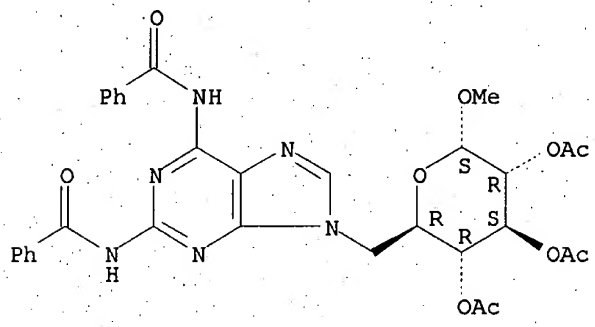
ACCESSION NUMBER: 1974:15149 HCAPLUS

DOCUMENT NUMBER: 80:15149

TITLE: Synthesis of reversed nucleosides of some purine and

pyrimidine bases
AUTHOR(S): Fukatsu, Shunzo; Takeda, Yoshiro; Umezawa, Sumio
CORPORATE SOURCE: Fac. Eng., Keio Univ., Hiyoshi, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1973), 46(10), 3165-8
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Me 5-(6-aminopurin-9-yl, Me 5-(uracil-1-yl)-, and Me 5-(cytosin-1-yl)-5-deoxy-.alpha.,.beta.-D-ribofuranoside and Me 6-(6-aminopurin-9-yl)-, Me 6-(2,6-diaminopurin-9-yl)-, Me 6-(uracil-1-yl)-, and Me 6-(cytosin-1-yl)-6-deoxy-.alpha.-D-glucopyranoside were prepd. by condensation of terminal iodo-sugars with purine and pyrimidine bases in DMF in the presence of NaH or LiH.
CC 33-7 (Carbohydrates)
IT 6304-96-7P 29781-12-2P 51173-47-8P 51173-48-9P 51173-49-0P
51173-50-3P 51173-51-4P 51173-52-5P 51173-53-6P 51173-54-7P
51173-55-8P 51173-56-9P **51173-58-1P** 51173-59-2P
51173-60-5P 51173-61-6P 51173-62-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **51173-58-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 51173-58-1 HCAPLUS
CN .alpha.-D-Glucopyranoside, methyl 6-[2,6-bis(benzoylamino)-9H-purin-9-yl]-6-deoxy-, 2,3,4-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 36 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1973:97600 HCAPLUS
DOCUMENT NUMBER: 78:97600
TITLE: Synthesis of purine derivatives. XXXII. Transformation of 2-R-1,9-dimethylhypoxanthines
AUTHOR(S): Ovcharova, I. M.; Golovchinskaya, E. S.
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1973), 7(1), 3-7
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.

AB Hypoxanthines (I; R = MeHN, PhCH2CHMeHN) were prepd. in 98% and 78% yields, resp., by amination of I (R = Cl) with the corresponding amine. Treatment of I (R = SH) with BuBr gave 80% hypoxanthine(I; R = BuS). Iminopurines (II; R = MeHN, EtHN, PhCH2CHMeHN), BuS, Me2N, Me) were prepd. in 39-70% yields by boiling the corresponding I with a 5-8-fold excess of POCl3. Treatment of I (R = Me2N, Et2N, Me) with a 10-fold excess of POCl3 gave the corresponding chloropurines III.

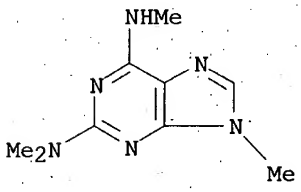
CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 40423-33-4P 40423-34-5P 40423-35-6P 40423-36-7P 40423-37-8P
40423-38-9P 40423-39-0P 40423-40-3P 40423-41-4P 40423-42-5P
40423-43-6P 40423-44-7P 40423-45-8P 40423-46-9P
40423-47-0P 40423-48-1P 40562-85-4P 40614-73-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **40423-43-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 40423-43-6 HCAPLUS

CN 9H-Purine-2,6-diamine, N2,N2,N6,9-tetramethyl- (9CI) (CA INDEX NAME)



L5 ANSWER 37 OF 40 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1972:99620 HCAPLUS

DOCUMENT NUMBER: 76:99620

TITLE: Facile synthesis of 9-alkylpurines. Preparation of some 9-ethylpurine derivatives

AUTHOR(S): Israel, Mervyn; Muhammad, Naseem; Modest, Edward J.

CORPORATE SOURCE: Child. Cancer Res. Found., Boston, MA, USA

SOURCE: Journal of Heterocyclic Chemistry (1971), 8(6), 1019-23
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Ethylation (EtI-K2CO3) of the thiopurine (I) gave the I 9-ethyl deriv. (II), which with NH3 gave 2,6-diamino-3-ethylpurine (III). Cleavage of the thioether function in II with CF3-CO2H-PhOH gave 2-amino-9-ethyl-6-purinethiol (IV), which with K2CO3-PhCH2Cl gave the IV S-benzyl deriv. (V) and with 1-methyl-4-nitro-5-chloroimidazole-NaOAc gave a IV S-(5-imidazolyl) deriv. (VI). Thiol IV was treated with Me2SO4 and then with BuNH2 to give IV 6-butylamino analog (VII); dethiation (Ni) of IV gave 2-amino-9-ethylpurine (VIII). Similarly, ethylation of 2,6-bis(diphenylmethylthio)purine and thioether cleavage gave 9-ethyl-2,6-purinedithiol (IX), which also gave 2,6-bis-(benzylthio) and 2,6-bis(5-imidazolylthio) derivs. (X and XI, resp.). Treating IX with MeI or EtI caused 2,3,6-trialkylation to the purinium iodides (XII or XIII, resp.).

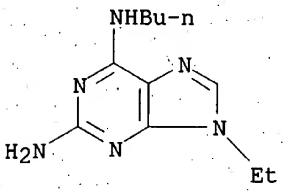
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 10320-82-8P 16417-68-8P 24397-94-2P 35549-08-7P 35549-11-2P
35549-12-3P **35549-13-4P** 35549-16-7P 35549-17-8P
35549-18-9P 35549-39-4P 35549-40-7P 35611-96-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

IT **35549-13-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 35549-13-4 HCAPLUS

CN 9H-Purine-2,6-diamine, N6-butyl-9-ethyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

L5 ANSWER 38 OF 40 HCAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1972:34213 HCAPLUS

DOCUMENT NUMBER: 76:34213

TITLE: New, general synthesis of 2-, 8-, and 9-substituted adenines

AUTHOR(S): Taylor, Edward Curtis; Beardsley, George P.; Maki, Yoshifumi

CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, USA

SOURCE: Journal of Organic Chemistry (1971), 36(21), 3211-17
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

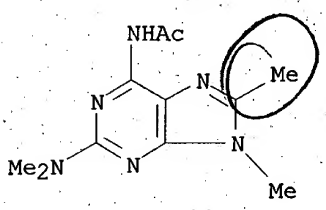
GI For diagram(s), see printed CA Issue.

AB A new synthesis of adenine derivs. involves the initial conversion of a 4,6-diamino-5-nitrosopyrimidine to a 7-aminofurazano[3,4-d]-pyrimidine (I, R=H, Me, Ph, NH2, MeS, Me2N) by Pb(OAc)4 oxidn., introduction of the eventual adenine 9- and 8-substituents by reaction of I with an alkylamine followed by acylation and reductive cleavage of the furazan ring to give an intermediate, 4-acylamino-5,6-diaminopyrimidine, which recyclizes to the desired adenine deriv. All reactions proceed under mild conditions, and all substituents are introduced unambiguously.

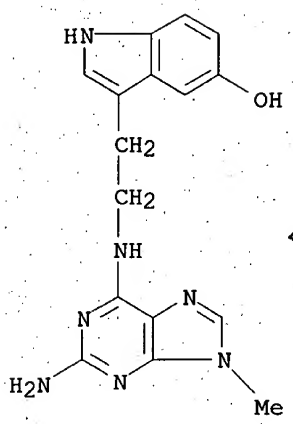
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))

IT 22003-13-0P 30708-66-8P 30708-67-9P 30708-68-0P 30720-36-6P
30720-37-7P 30720-38-8P 30720-39-9P 30720-40-2P 30720-41-3P
30720-42-4P 30720-43-5P 30720-44-6P 30720-45-7P 30720-46-8P
30720-47-9P 30720-48-0P 30720-49-1P 30720-50-4P 30720-51-5P
30720-52-6P 30720-53-7P 30720-54-8P 30720-55-9P 30720-56-0P
30720-57-1P 30720-58-2P 30720-59-3P 30720-60-6P 30720-61-7P
30720-62-8P 30720-63-9P 30720-64-0P 30720-65-1P 30720-66-2P
30720-67-3P 30720-68-4P **30720-69-5P** 30720-70-8P
30720-71-9P 30720-72-0P 30720-73-1P 30720-74-2P 30720-75-3P

30720-76-4P 30720-77-5P 30720-78-6P 30720-79-7P 30720-80-0P
30720-81-1P 30720-82-2P 30720-83-3P 30720-84-4P 30724-62-0P
30724-63-1P 30724-64-2P 30724-65-3P 30745-07-4P 30787-98-5P
30787-99-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **30720-69-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 30720-69-5 HCAPLUS
CN Acetamide, N-[2-(dimethylamino)-8,9-dimethyl-9H-purin-6-yl]- (9CI) (CA INDEX NAME)



L5 ANSWER 39 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1969:4056 HCAPLUS
DOCUMENT NUMBER: 70:4056
TITLE: Synthesis of potentially antiblastic substances related to 5-hydroxytryptamine (serotonin). III. Products of the condensation of serotonin with some purine derivatives
AUTHOR(S): Petrova, M. F.; Kozhevnikova, I. V.; Kaverina, N. S.; Golovchinskaya, E. S.; Pukhal'skaya, E. Ch.; Men'shikov, G. P.
CORPORATE SOURCE: Inst. Eksp. Klin. Onkol., Moscow, USSR
SOURCE: Puti Sin. Izyskaniya Protivoopukholevykh Prep., Tr. Simp., 2nd, Moscow (1967), Meeting Date 1965, 150-2. Editor(s): Berlin, A. Ya. Izdatel'stvo "Meditsina": Moscow, USSR.
CODEN: 20BOAD
DOCUMENT TYPE: Conference
LANGUAGE: Russian
GI For diagram(s), see printed CA Issue.
AB Serotonin (I) was condensed with purine (II) derivs. contg. Cl in the position 6 to yield III, IV, V, and VI, m. 244-6.degree., 208-10.degree., 240-2.degree., and 255-7.degree., resp. The compds. had no antiblastic activity. II derivs. with Cl in the position 2 did not react with I. Compds. with Cl in the aliphatic chain did not give cryst. products.
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 20914-54-9P 20914-64-1P 20914-65-2P **21184-29-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **21184-29-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 21184-29-2 HCAPLUS
CN Indol-5-ol, 3-[2-[(2-amino-9-methyl-9H-purin-6-yl)amino]ethyl]- (8CI) (CA INDEX NAME)



-Not provisoed wt by odd proviso

L5 ANSWER 40 OF 40 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1967:508955 HCAPLUS
DOCUMENT NUMBER: 67:108955
TITLE: Purine nucleosides
INVENTOR(S): Honjo, Mikio; Imai, Kinichi
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd.
SOURCE: Jpn. Tokkyo Koho, 3 pp.
CODEN: JAXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 42010519	B4	19670607	JP	19650205

AB 1-O-Acetyl-2,3,5-tri-O-benzoyl-.beta.-D-ribofuranose (5 g.) is heated at 140-50.degree., 1.38 g. 2,6-diacetamido-9-acetylpurine and 200 mg. iodine are added, the mixt. heated at 170-5.degree. for 5 min. then at the same temp. in vacuo for 15 min., cooled, extd. with 100 ml. CHCl3, the ext. evapd., the residue refluxed 1 hr. in 70 ml. with 1% MeONa, neutralized with AcOH, concd. in vacuo, the residue is made alk. with N NH4OH, passed through a column of Dowex-1 (Cl form) (100-200 mesh), and the column is eluted with 0.01M NH4Cl buffer (pH 10.5) to give 792 mg. 2,6-diacetamido-9-acetylpurine, m. 238.degree. (H2O). Similarly prepd. are 7-(.beta.-D-ribofuranosyl)theophylline, m. 188-90.degree., 2,6-dichloro-9-(tri-O-acetyl-.beta.-D-ribofuranosyl)purine (sirup), adenosine, and inosine.

NCL 16E611.2
CC 33 (Carbohydrates)
IT 2096-10-8P 3056-18-6P 3624-44-0P **17601-00-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
IT **17601-00-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 17601-00-2 HCAPLUS
CN Acetamide, N,N'-(9-acetyl-9H-purine-2,6-diyl)bis- (8CI, 9CI) (CA INDEX

NAME)